Université de Lille

iemn
Institut d'Electronique, de Microélectronique et de Nanotechnologie
UMR CNRS 8520

INDIAN INSTITUTE OF TECHNOLOGY, ROORKEE

Numerical method to simulate soluble surfactants

University of Lille - Institute of Electronics, Microelectronics and Nanotechnology

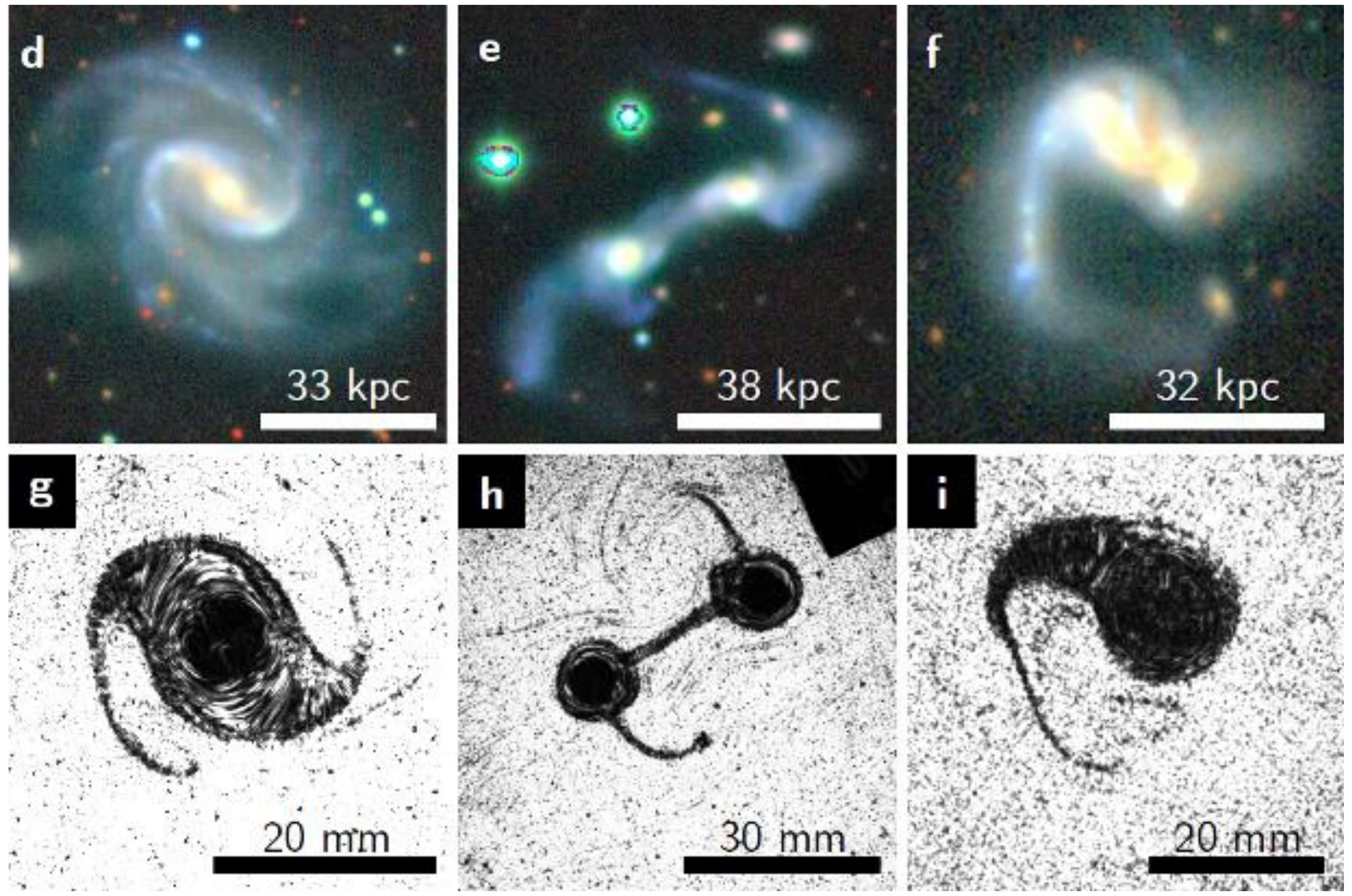
Basilisk (Gerris) Users' Meeting 2025

Ilies Haouche, Palas Kumar Farsoiya & Michaël Baudoin

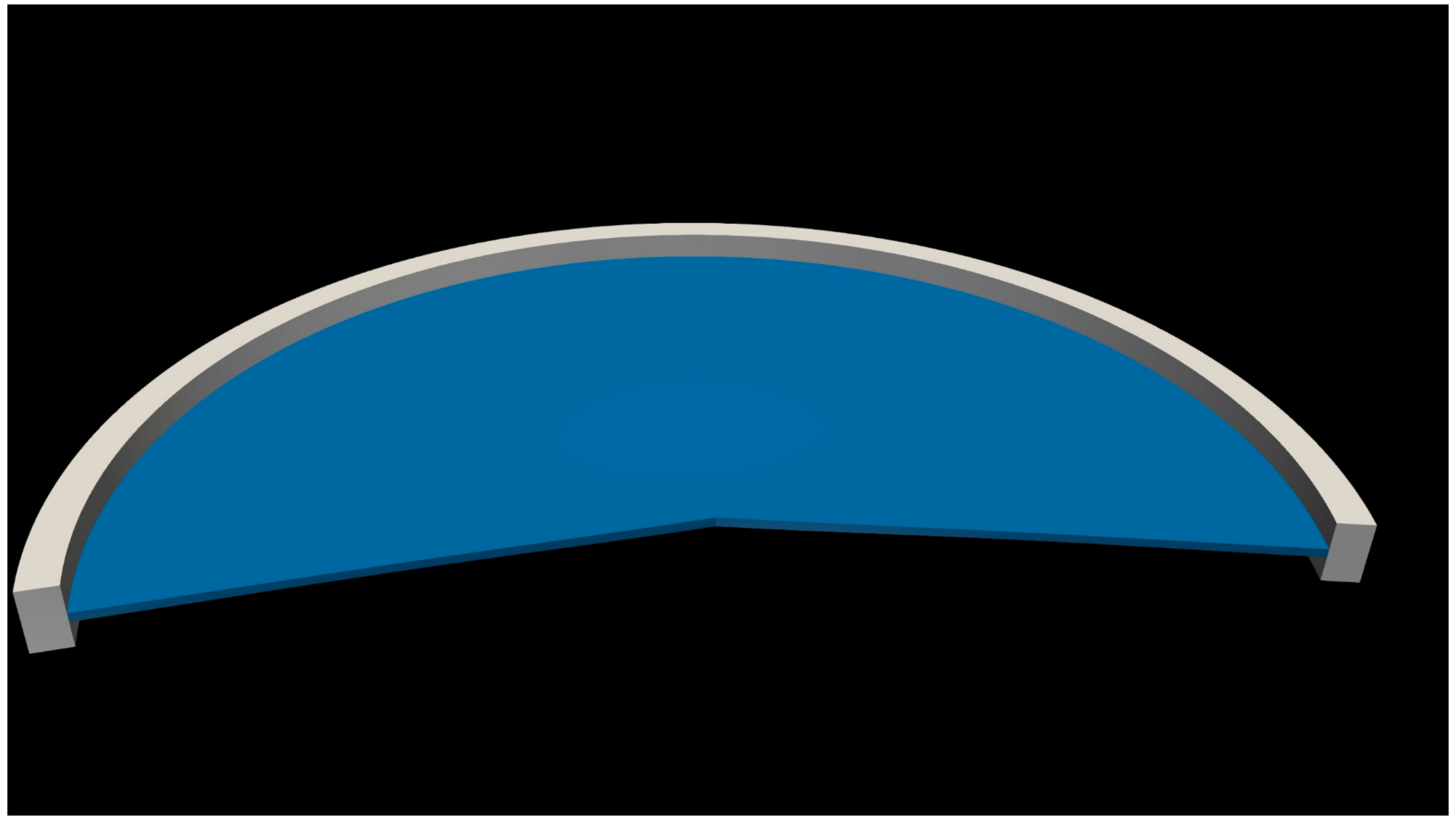
cnrs

Motivation

Made by Jean-Paul Martishang

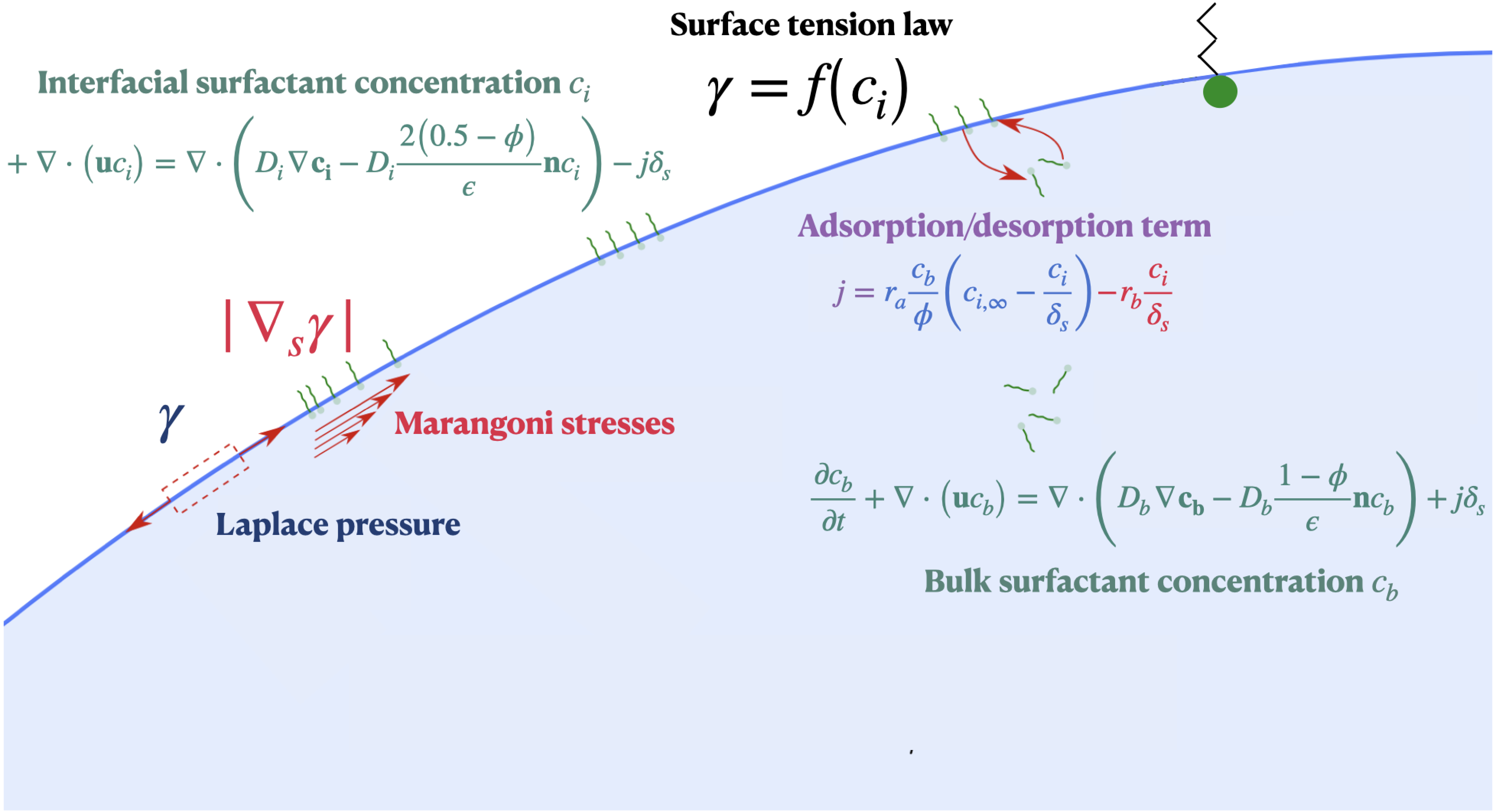


J. P. Martishang, B. Reichert, I. Haouche, G. Rousseaux, A. Duchesne, M. Baudoin« *Orbiting, colliding and merging droplets on a soap film: toward gravitational analogues* » submitted



Simulation from Basilisk

What is surfactant?



Surface tension law

$$\gamma = f(c_i)$$

Interfacial surfactant concentration c_i

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u}c_i) = \nabla \cdot \left(D_i \nabla \mathbf{c_i} - D_i \frac{2(0.5-\phi)}{\epsilon} \mathbf{n} c_i \right) - j\delta_s$$

Adsorption/desorption term

$$j = r_a \frac{c_b}{\phi} \left(c_{i,\infty} - \frac{c_i}{\delta_s} \right) - r_b \frac{c_i}{\delta_s}$$

$$|\nabla_s \gamma|$$

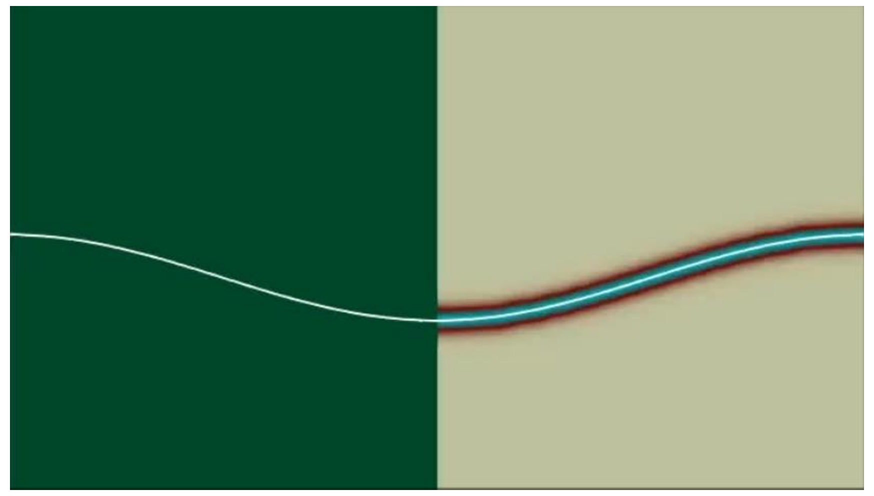
$$\gamma$$

Marangoni stresses

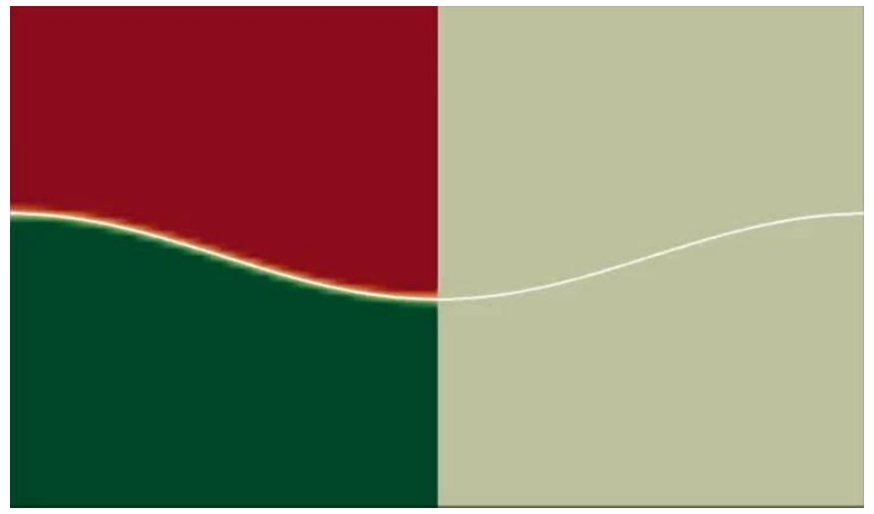
Laplace pressure

$$\frac{\partial c_b}{\partial t} + \nabla \cdot (\mathbf{u}c_b) = \nabla \cdot \left(D_b \nabla \mathbf{c_b} - D_b \frac{1-\phi}{\epsilon} \mathbf{n} c_b \right) + j\delta_s$$

Bulk surfactant concentration c_b



Desorption



Adsorption

Why is it a challenge to compute them?

	2D	2D-Axi	3D	AMR	Open-source
S. S. Jain (2023)	✅	❌	❌	❌	❌
Muradoglu et al., Journal of Comp. Phys. (2008)	✅	❌	❌	❌	❌
Teigen et al., Journal of Comp. Phys. (2011)	✅	❌	✅	✅	❌
Atasi et al., Langmuir (2018)	❌	✅	❌	❌	❌
Campana et al., Phys. Fluid (2006)	✅	✅	❌	❌	❌
Constante-Amores et al., Jour. Fluid. Mech (2020)	❌	❌	✅	❌	❌
Craster et al., Rev. Modern Physics (2009)	✅	✅	❌	❌	❌
Present work	✅	✅	✅	✅	✅

Governing equations

- Flow part:

Navier-Stokes equations:

$$\rho(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \nabla \cdot (\mu(\nabla \mathbf{u} + \nabla^T \mathbf{u})) + \gamma \kappa \delta_s \mathbf{n} + \delta_m \nabla_s \gamma \mathbf{t}$$

$$\nabla \cdot \mathbf{u} = 0$$

- Interface part:

VoF method:

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = 0$$

Phase field method:

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = \nabla \cdot (\zeta(\epsilon \nabla \phi - \frac{1}{4}[1 - \tanh^2(\frac{\psi}{2\epsilon})] \frac{\nabla \psi}{|\nabla \psi|}))$$

$$\psi = \epsilon \log(\frac{\phi + \varepsilon}{1 - \phi + \phi})$$

- Surfactants part:

Bulk surfactant concentration $c_{b:}$:

$$\frac{\partial c_b}{\partial t} + \nabla \cdot (\mathbf{u} c_b) = \nabla \cdot (D_b \nabla \mathbf{c_b} - D_b \frac{1 - \phi}{\epsilon} \mathbf{n} c_b) + j \delta_s$$

Interfacial surfactant concentration c_i:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (\mathbf{u} c_i) = \nabla \cdot (D_i \nabla \mathbf{c_i} - D_i \frac{2(0.5 - \phi)}{\epsilon} \mathbf{n} c_i) - j \delta_s$$

Adsorption term $j = r_a \frac{c_b}{\phi} (c_{i,\infty} - \frac{c_i}{\delta_s}) - r_b \frac{c_i}{\delta_s}$ Desorption term

S. S. Jain, « *Modeling soluble surfactants in two-phase flows* », (2023)

Solvers used

- Poisson.h —> $\nabla \cdot (\alpha \nabla a) + \lambda a = b$
- Diffusion.h —> $\theta \frac{\partial f}{\partial t} = \nabla \cdot (D \nabla f) + \beta f + r$
- Henry.h —> $\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c + \beta c)$
- Tracer.h —> $\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = 0$

- Strategy: Combine Diffusion.h with Tracer.h and Henry.h using Poisson.h
- Problem: Need a source term, we need to implement λ in the Henry.h

Time discretisation

- Euler implicit method for the diffusion and source terms:

$$\frac{d\mathbf{u}}{dt} = f(\mathbf{u}, t) \Rightarrow \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n}}{\Delta t} = f(\mathbf{u}^{n+1}, t_{n+1})$$

- Euler explicit for the advection term:

$$\frac{d\mathbf{u}}{dt} = f(\mathbf{u}, t) \Rightarrow \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n}}{\Delta t} = f(\mathbf{u}^{n}, t_{n})$$

Space discretisation

- Finite volume method with constant grid and AMR:

$$u_i = \frac{1}{\Delta} \int_K u(\mathbf{x}, t) dV$$

- Have to solve a conservative equation:

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F}(u) = 0$$

Courant-Friedrichs-Lewy criterion

$$\boxed{\Delta x \leq \frac{2D}{|u|_{max} + \frac{D}{\epsilon}}}$$

$$\Delta t \leq min(\Delta t_{conv}, \Delta t_{diff})$$

$$\Delta t_{conv} = \frac{\Delta x}{u_{eff}} \leq 1 \qquad \Delta t_{diff} = \frac{\Delta x^2}{2D} \leq \frac{1}{2}$$

$$\frac{\Delta x}{u_{eff}} \geq \frac{\Delta x^2}{2D} \Rightarrow \Delta x \leq \frac{2D}{u_{eff}} = \frac{2D}{|u|_{max} + \frac{D}{\epsilon}}$$

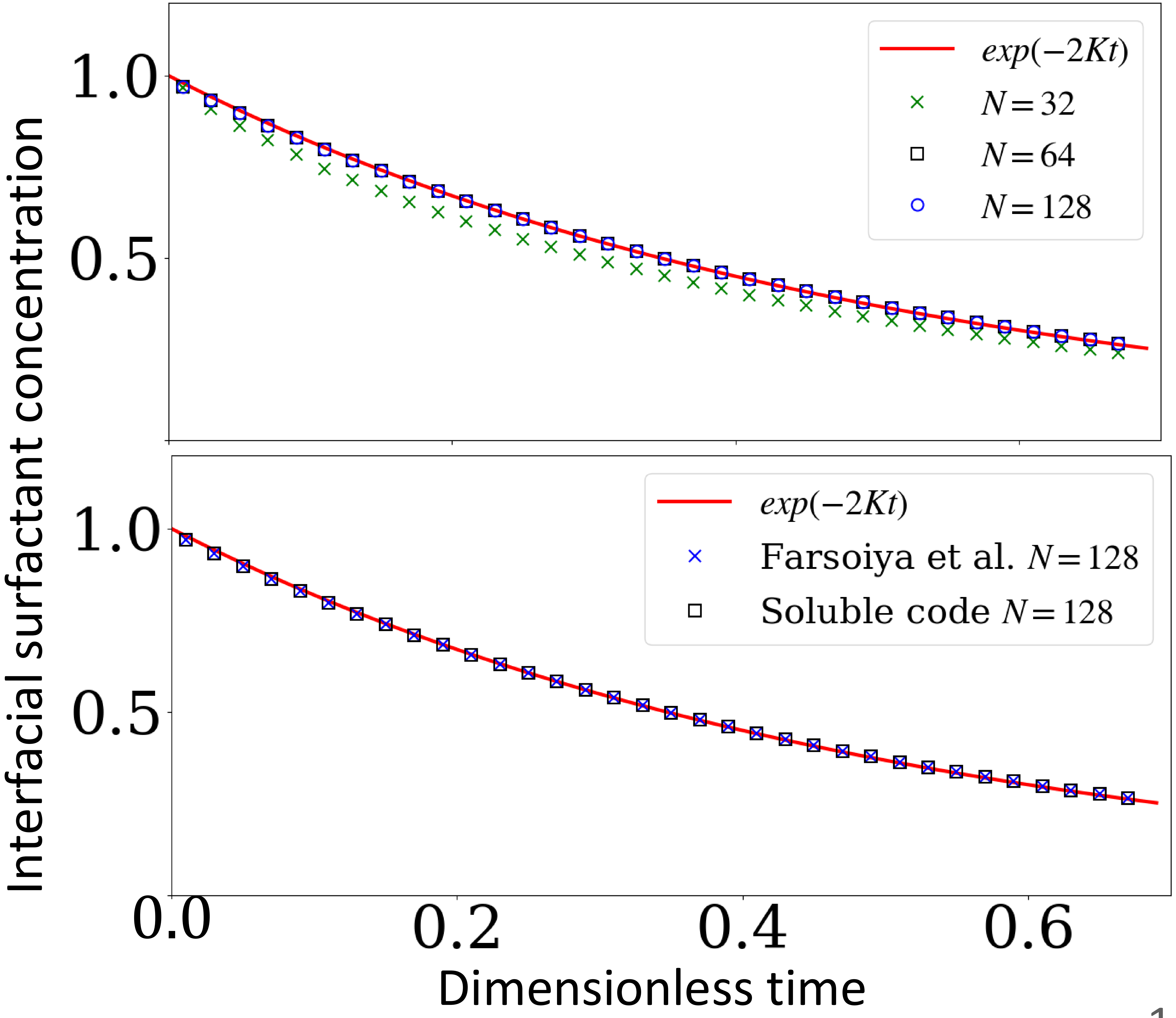
$$u_{eff} = \underbrace{|u|_{max}}_{\text{Convective term}} + \underbrace{\frac{D}{\epsilon}}_{\text{Anti-diffusion term}}$$

$$\boxed{\Delta t \leq \frac{\Delta x^2}{2N_d D}}$$

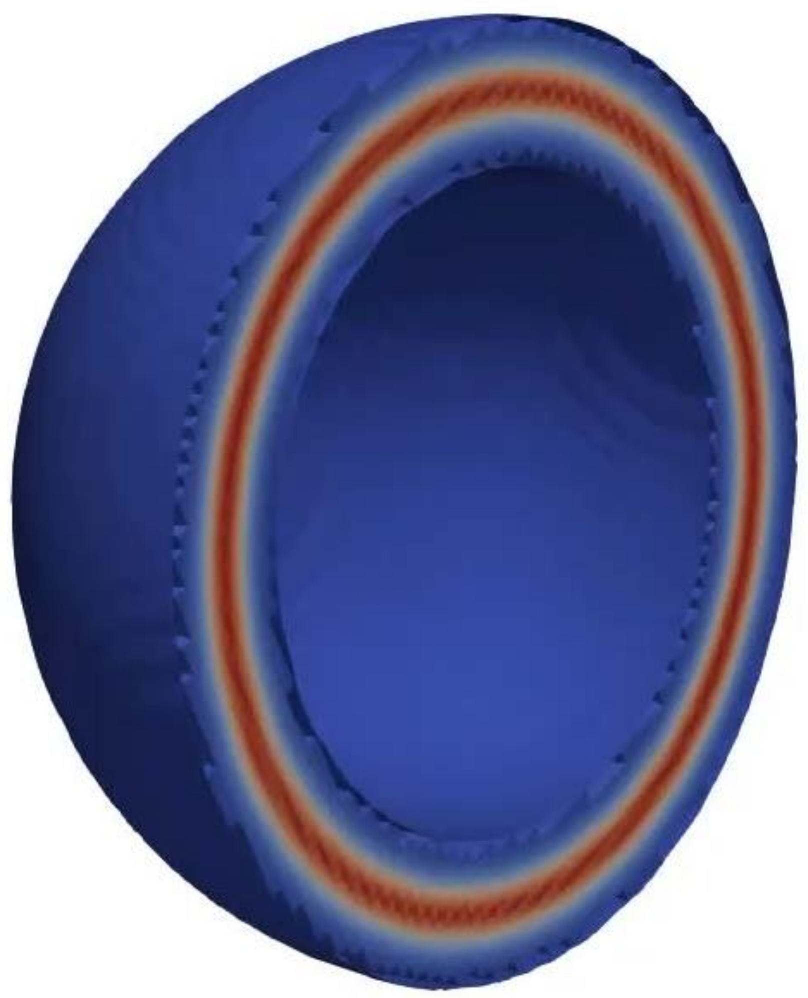
Test cases

Comparisons with analytical solutions

Expanding circle 3D



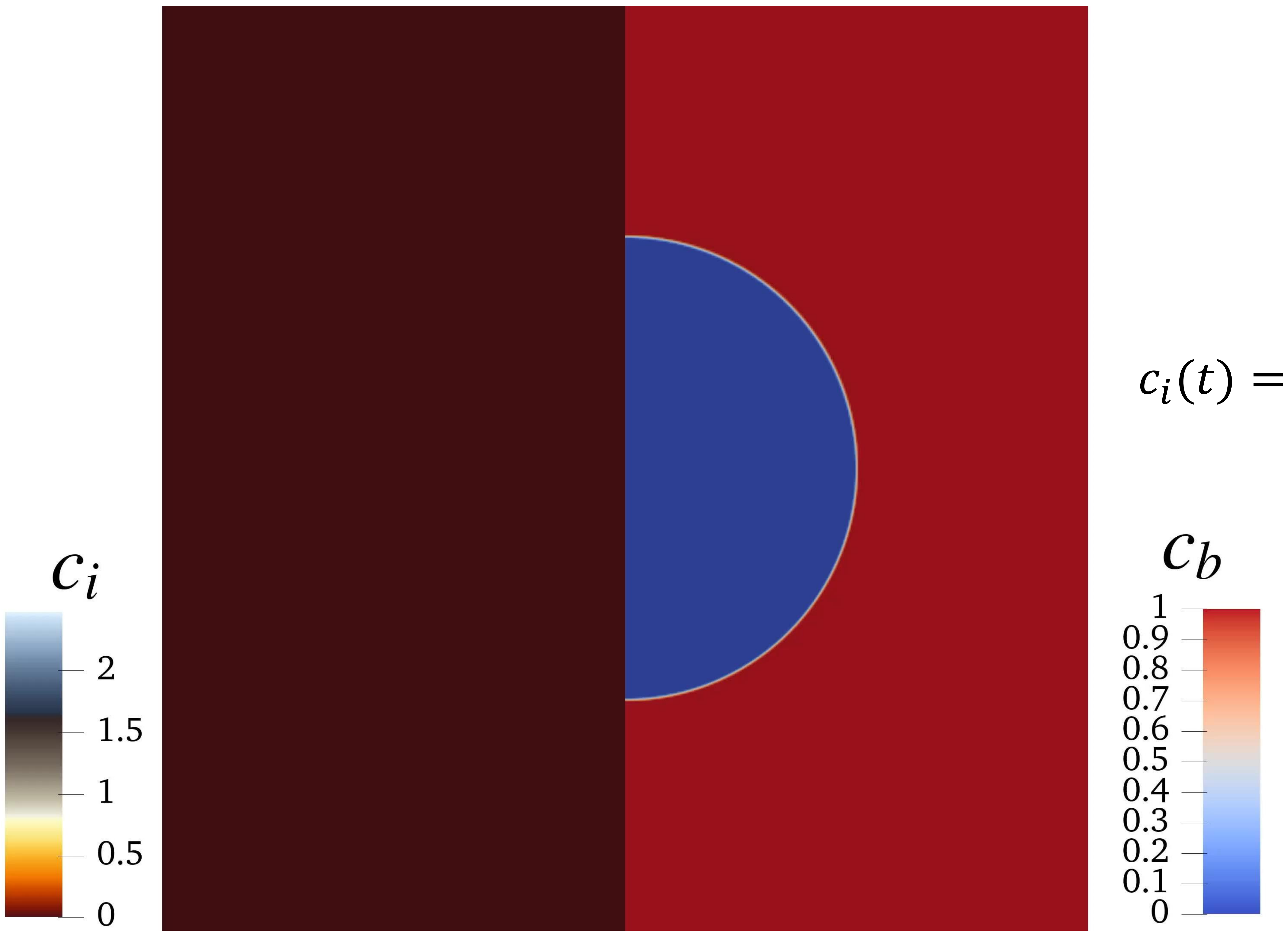
$$c_i(t) = c_i(0)e^{-2Kt}$$



Farsoiya et al., « *Coupled volume of fluid and phase field method for direct numerical simulation of insoluble surfactant-laden interfacial flows and application to rising bubbles* », Phys. Fluids (2024)

H. A. Stone, « *A simple derivation of the time-dependent convective-diffusion equation for surfactant transport along a deforming interface* », Phys. Fluids (1990)

Surfactant adsorption 2D

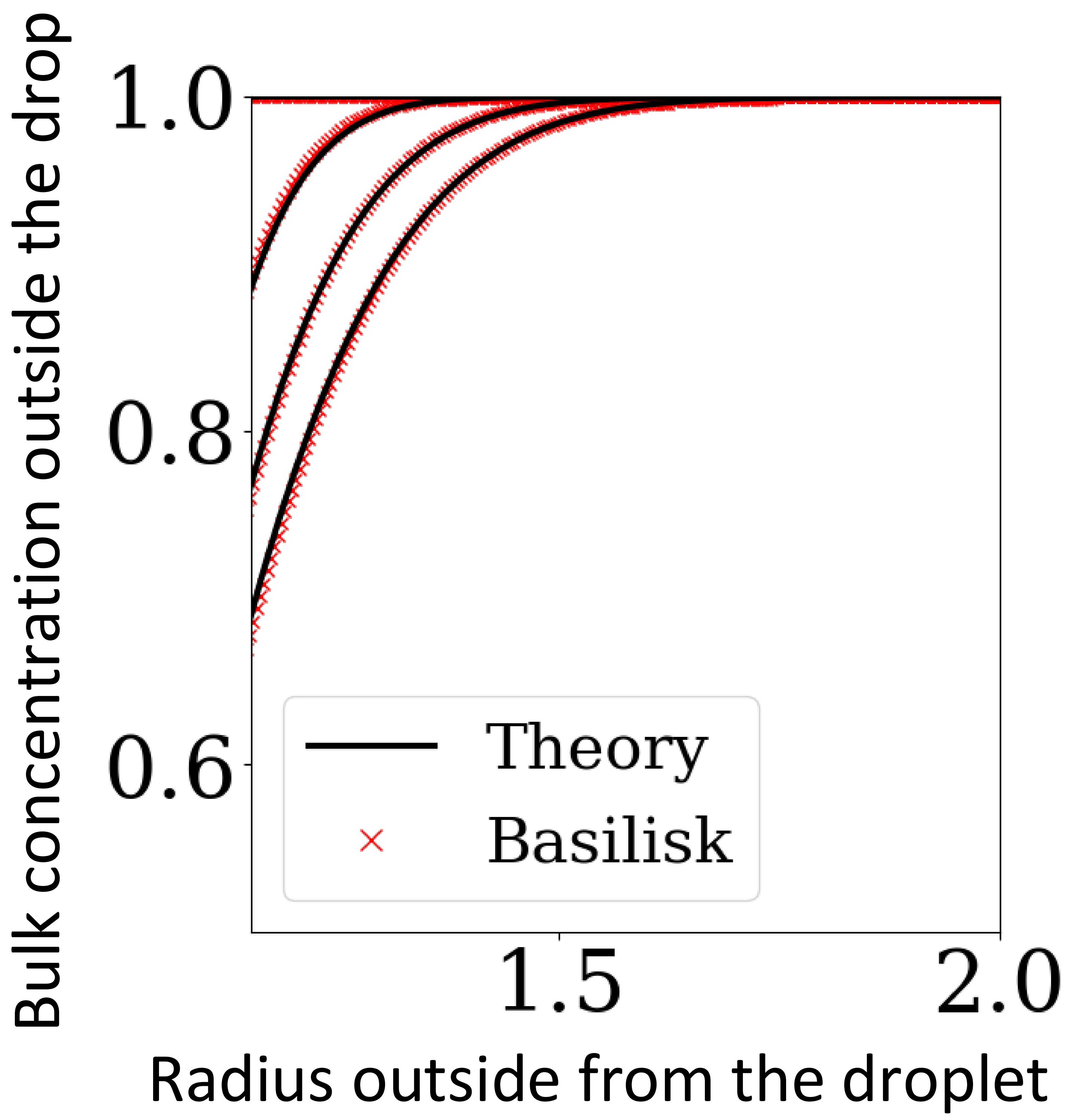


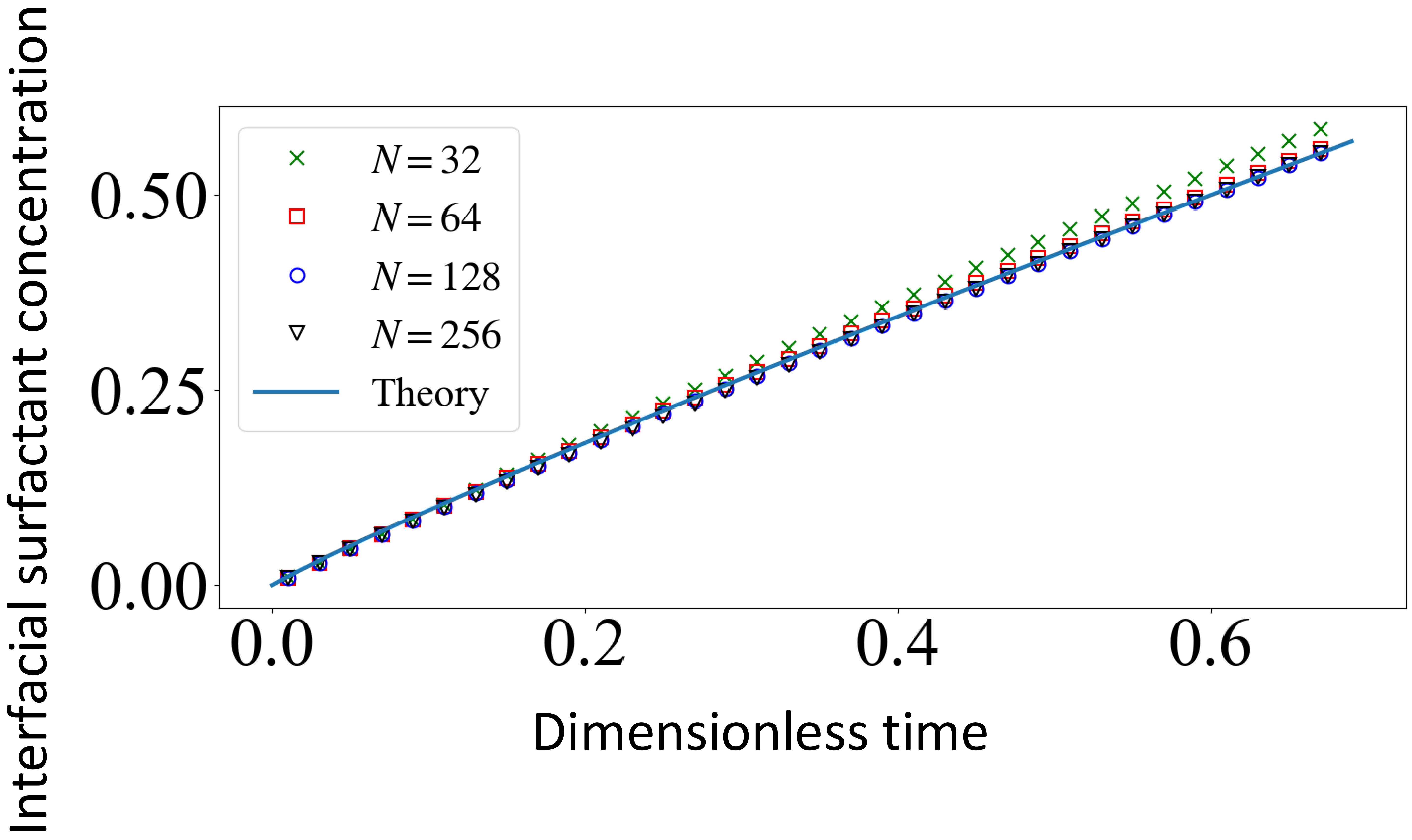
$$\frac{c_{b,\infty}-c_b(r,t)}{c_{b,\infty}} = \frac{r_a\sqrt{\pi D_i t}/D_i}{1+\frac{\sqrt{\pi D_i t}}{a}(1+\frac{a r_a}{D_i})}\frac{a}{r}\mathrm{erfc}\left(\frac{r-a}{2\sqrt{D_i t}}\right)$$

$$c_i(t) = c_i(0) + r_a c_{b,\infty}(t - \frac{\omega h}{\eta^3}(\eta^2 t - 2\eta\sqrt{t} + 2\log(1+\eta\sqrt{t})))$$

No surfactant can enter inside the droplet

Surfactant adsorption 2D





Muradoglu et al., « *A front-tracking method for computation of interfacial flows with soluble surfactants* », Journal Comp. Phys., (2008)

Test cases

Qualitative analysis without comparison with analytical solutions

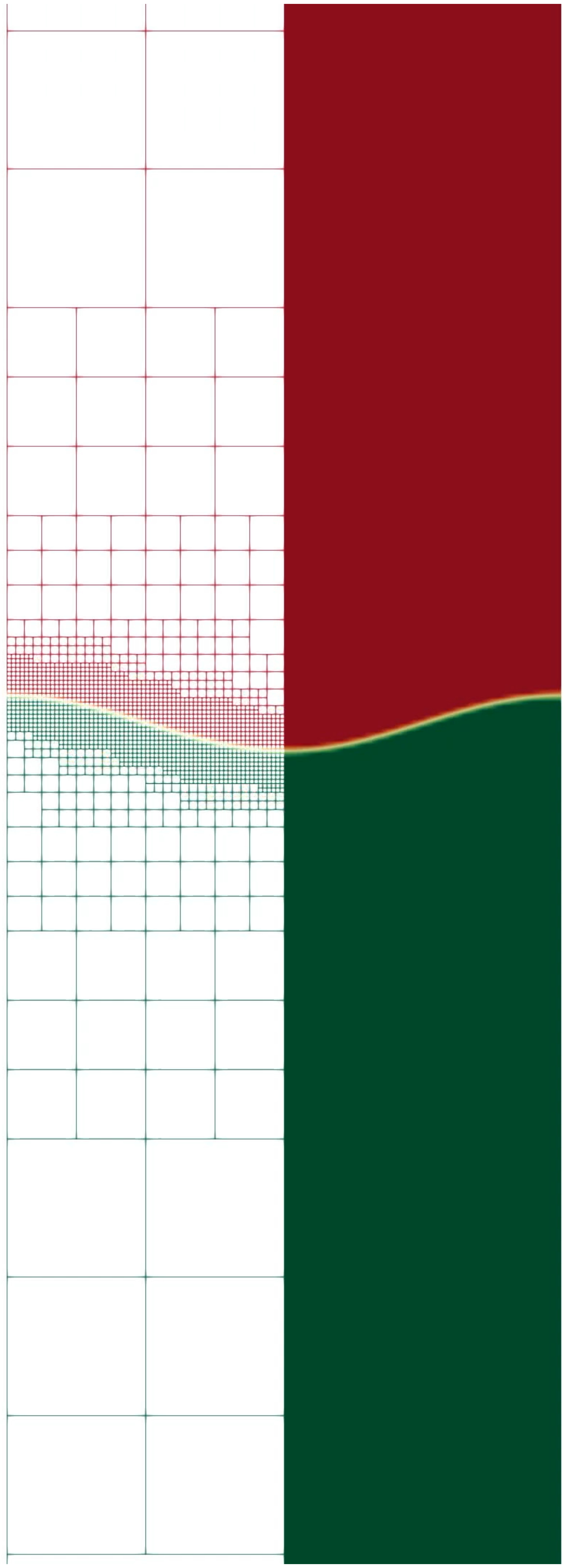
Rayleigh-Taylor instability 2D

$$\mathrm{Bo} = \frac{\textit{gravitational effect}}{\textit{capillary effect}} = \frac{\rho_l g L^2}{\gamma_0}$$

$$\mathrm{Oh} = \frac{\textit{viscous effect}}{\textit{inertial}-\textit{capillary effect}} = \frac{\mu_l}{\sqrt{\rho_l \gamma_0 L}}$$

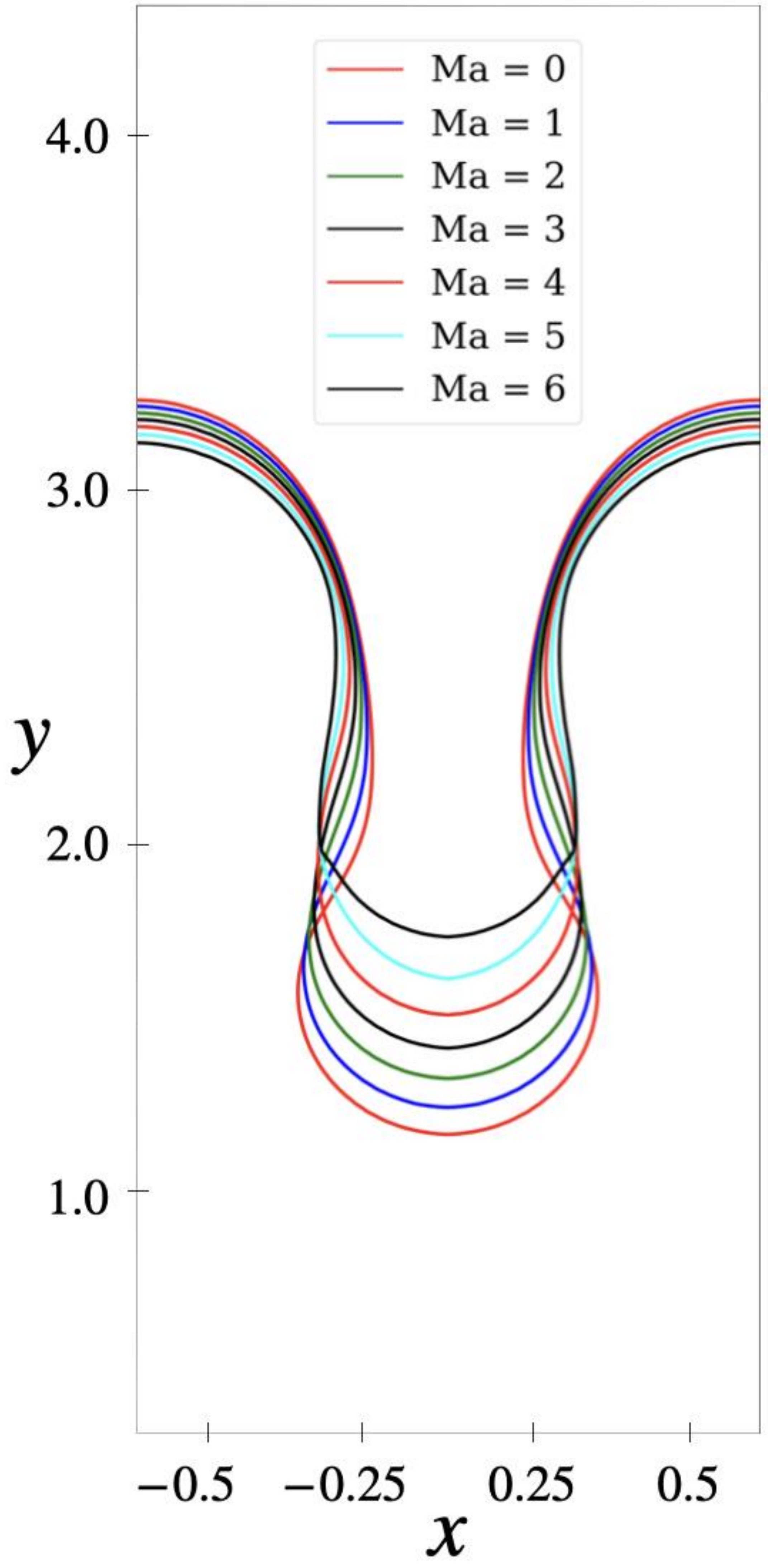
$$\mathrm{Pe} = \frac{\textit{convective effect}}{\textit{diffusive effect}} = \frac{UL}{D}$$

$$\mathrm{Ma} = \frac{\textit{shear force due to}\nabla\gamma}{\textit{diffusive effect}} = \frac{\beta\gamma_0}{\mu_l U}$$

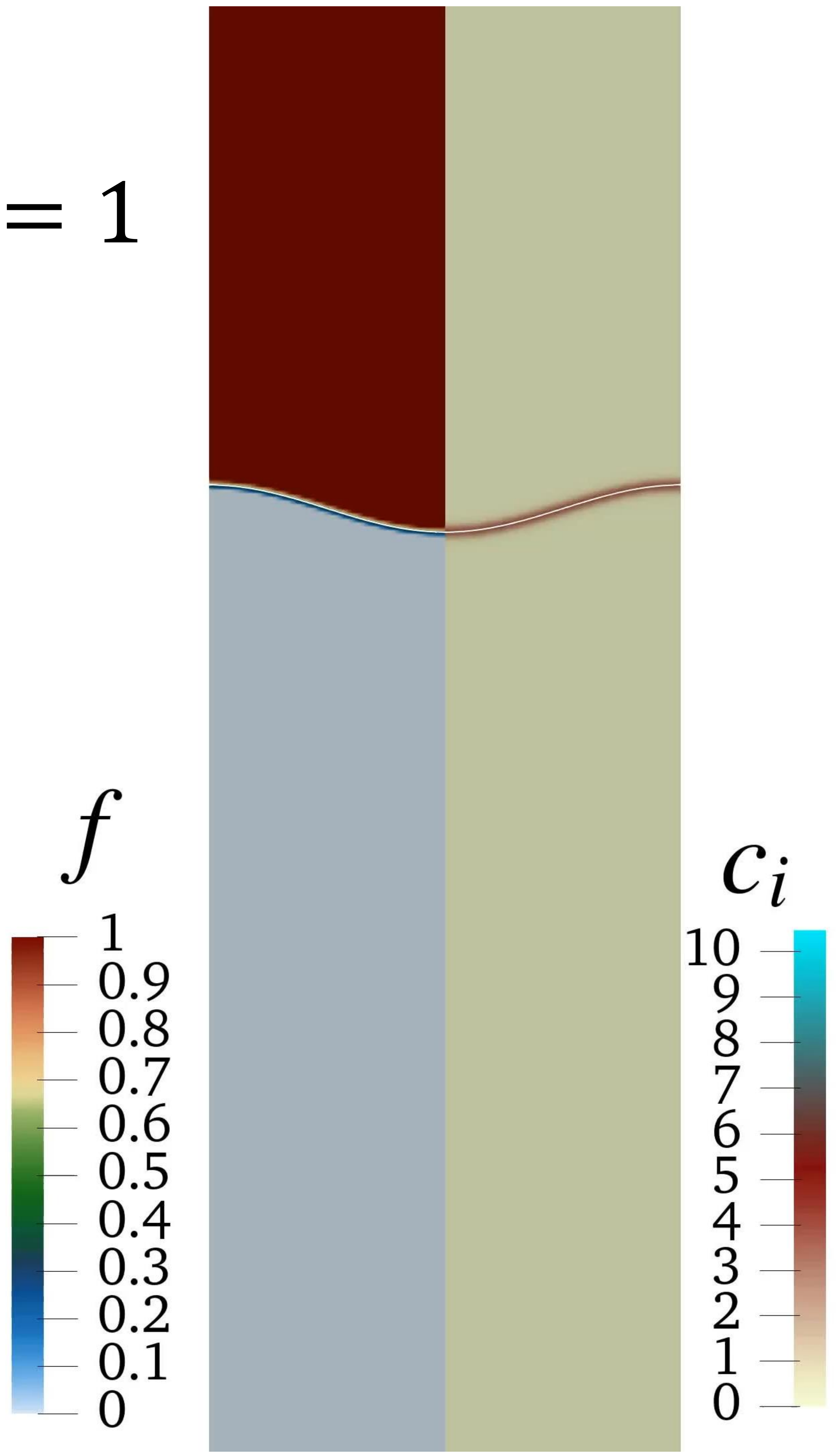


Rayleigh-Taylor instability 2D

Influence of the the Marangoni number with insoluble surfactants on the Rayleigh-Taylor instability

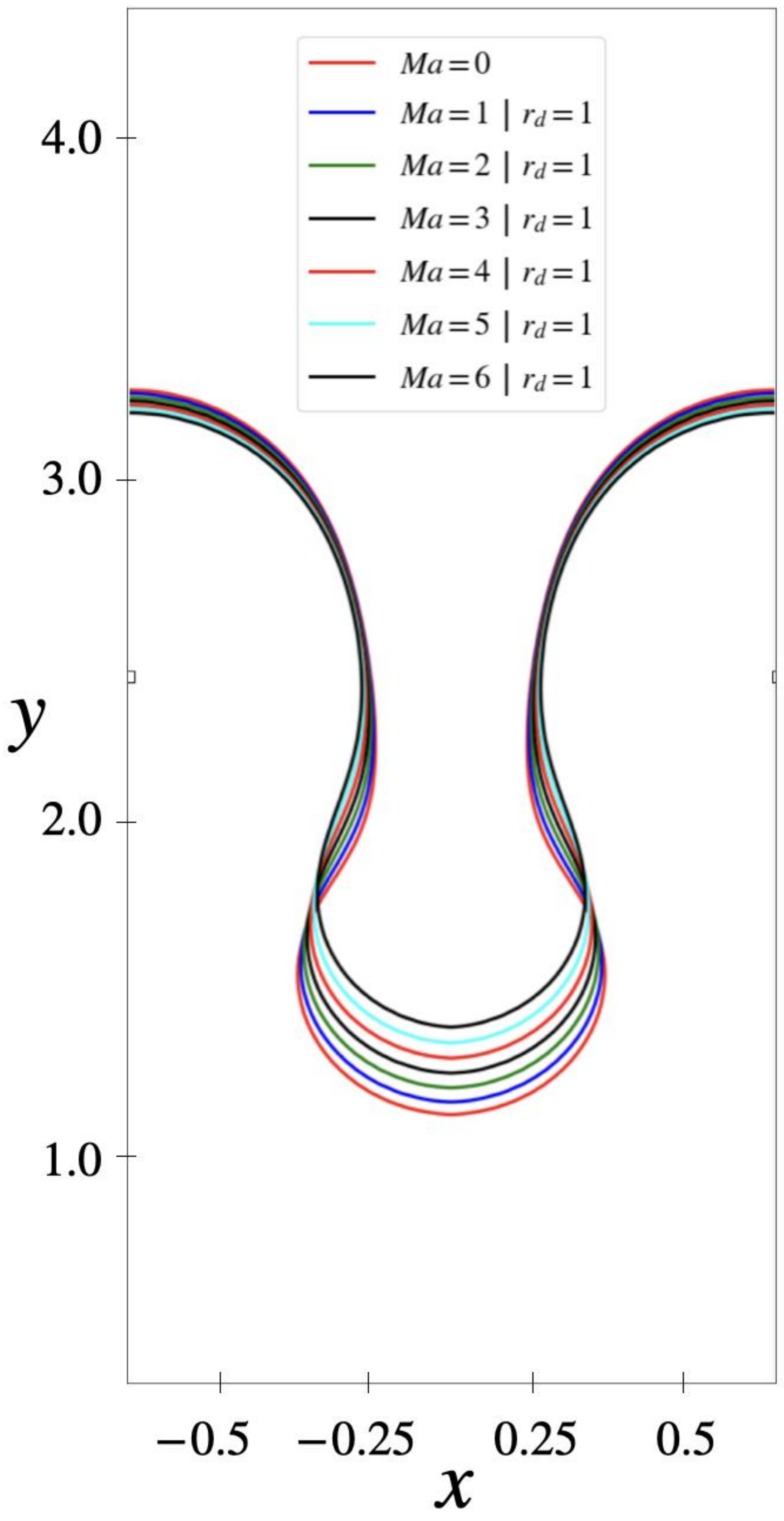


$Ma = 1$



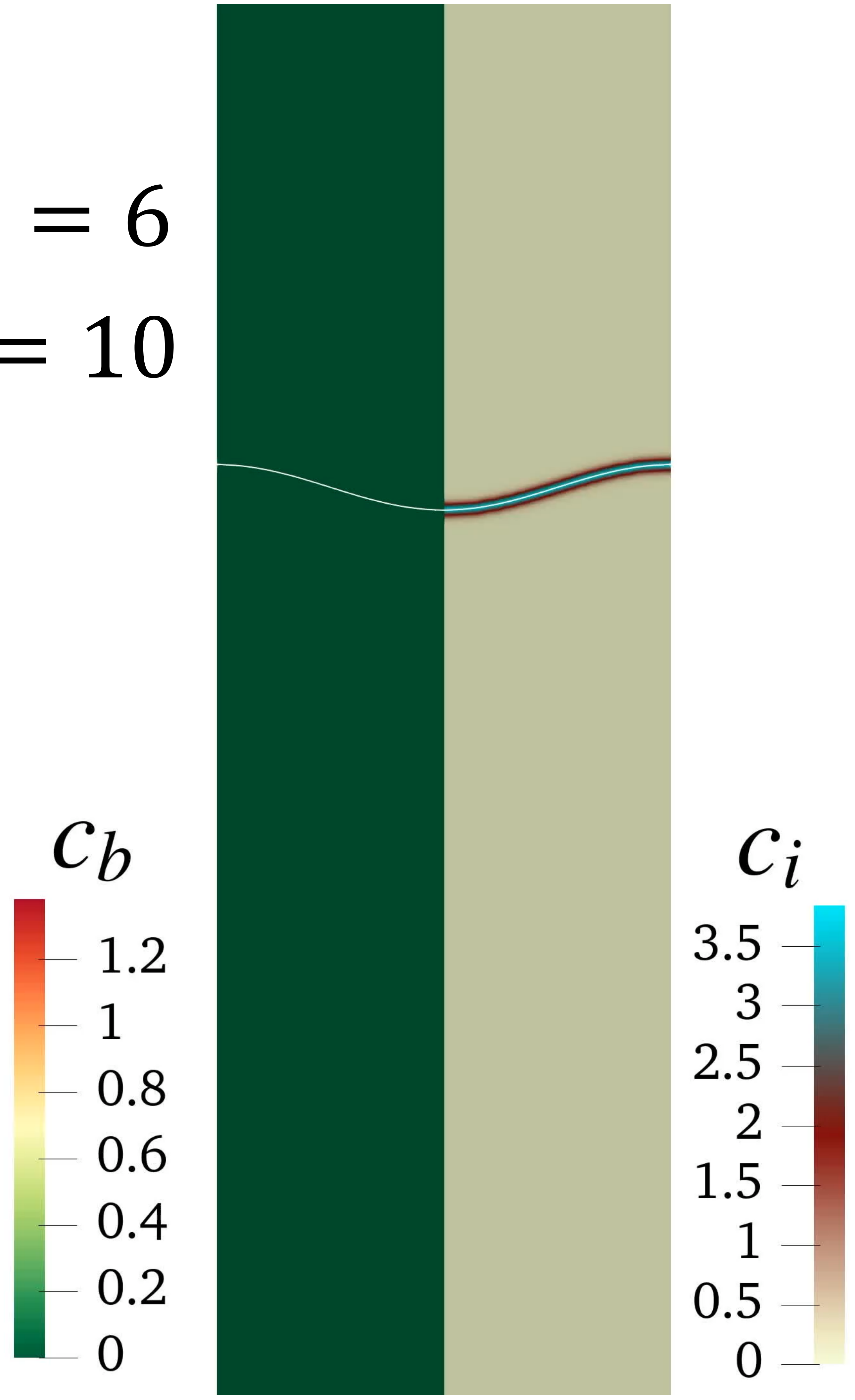
Rayleigh-Taylor instability 2D

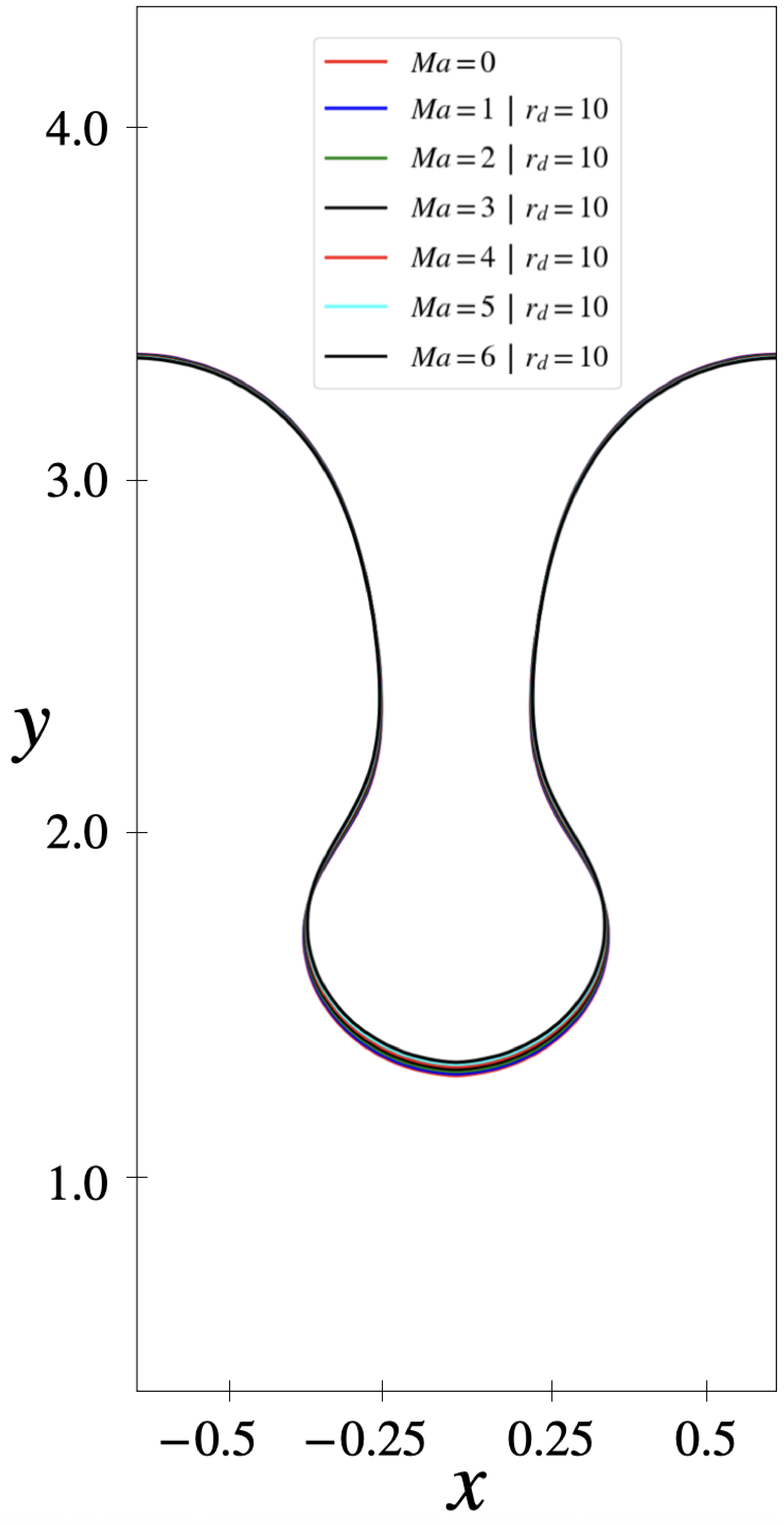
Influence of the the Marangoni number and the desorption on the Rayleigh-Taylor instability



$Ma = 6$

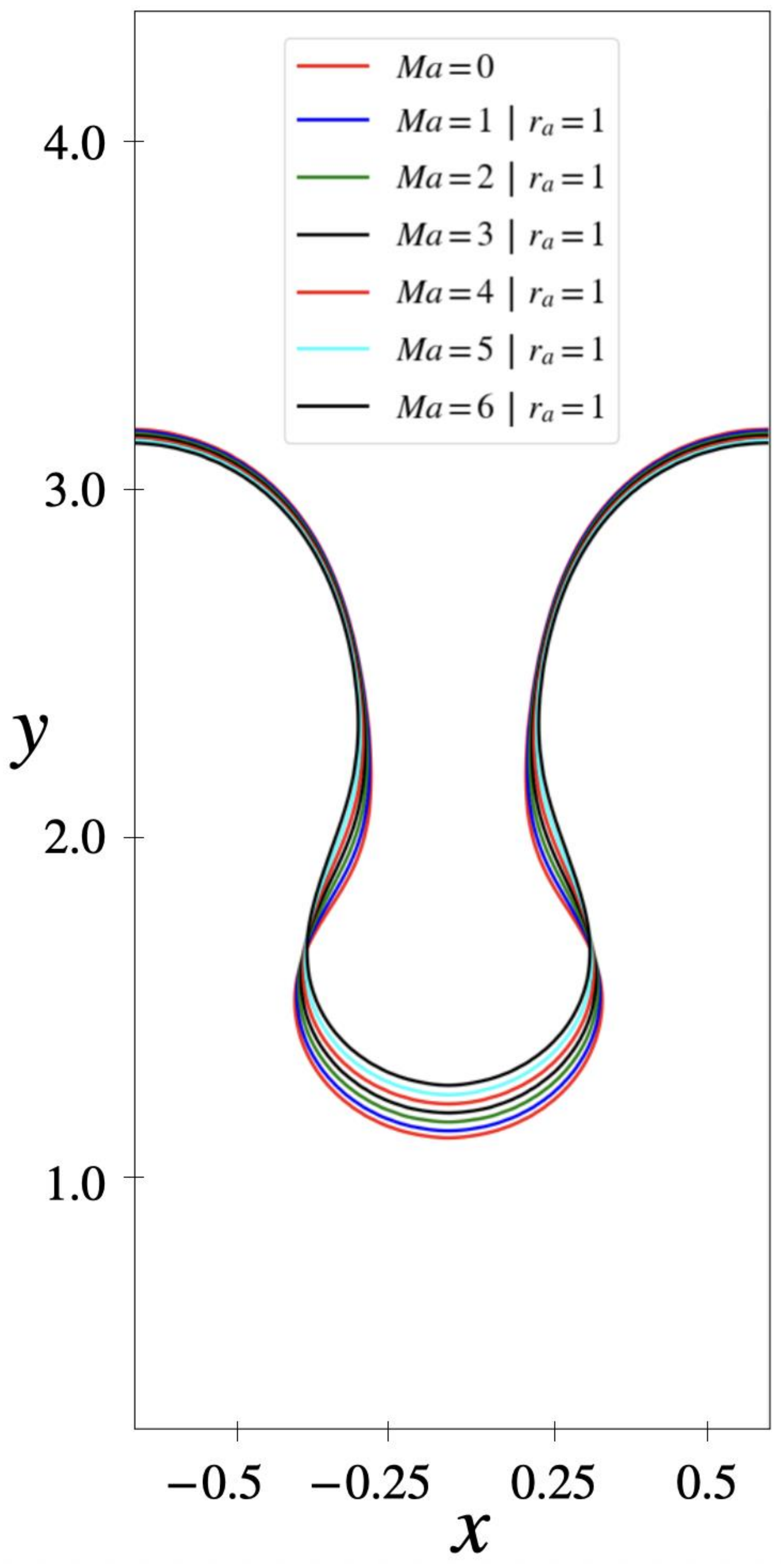
$r_d = 10$



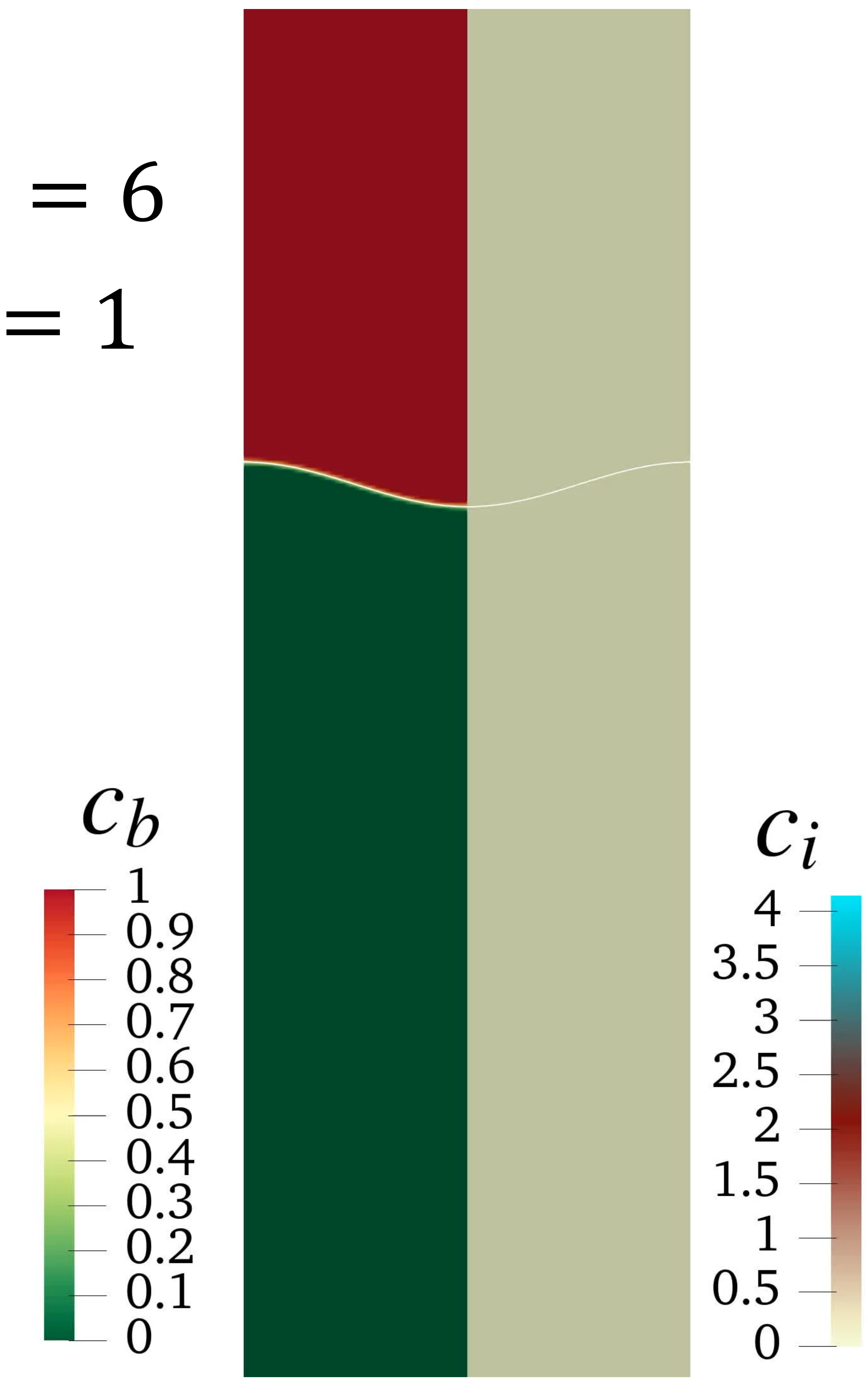


Rayleigh-Taylor instability 2D

Influence of the the Marangoni number and the adsorption on the Rayleigh-Taylor instability

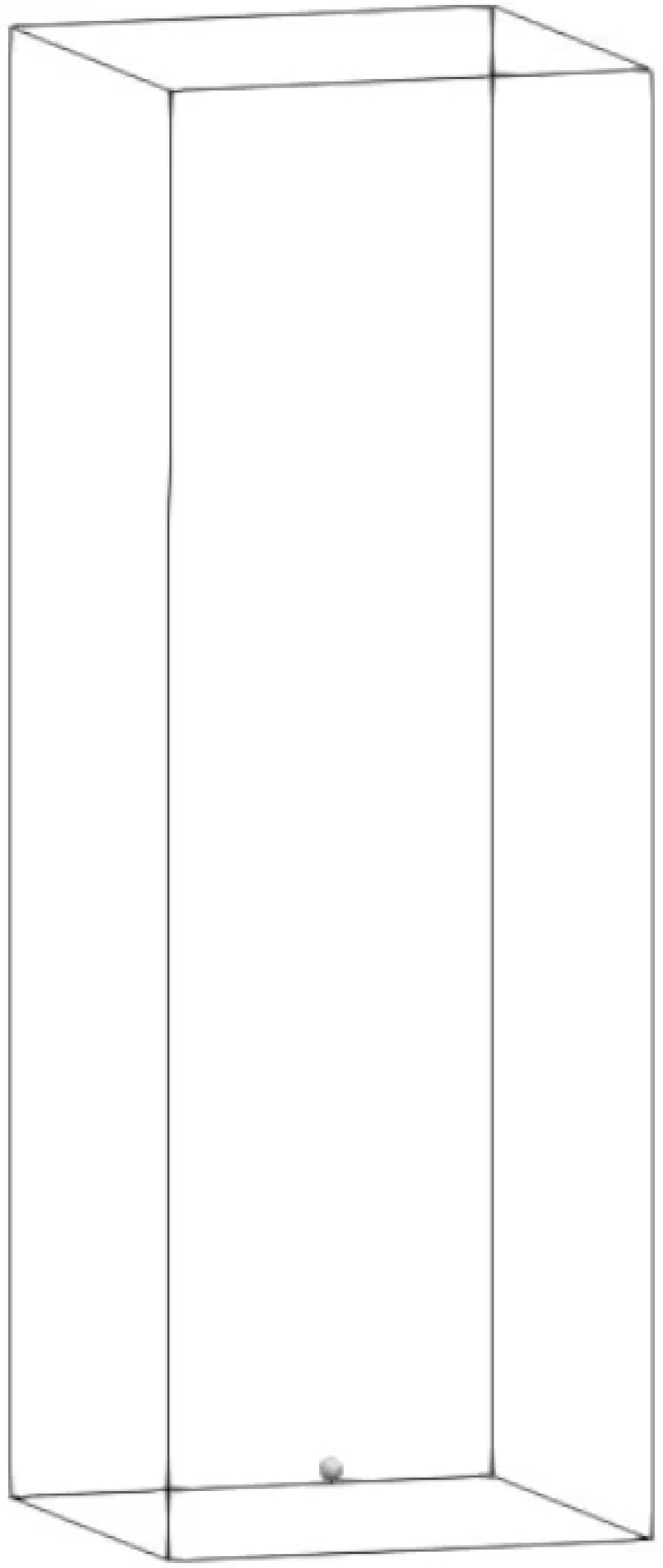


$$Ma = 6$$
$$r_a = 1$$



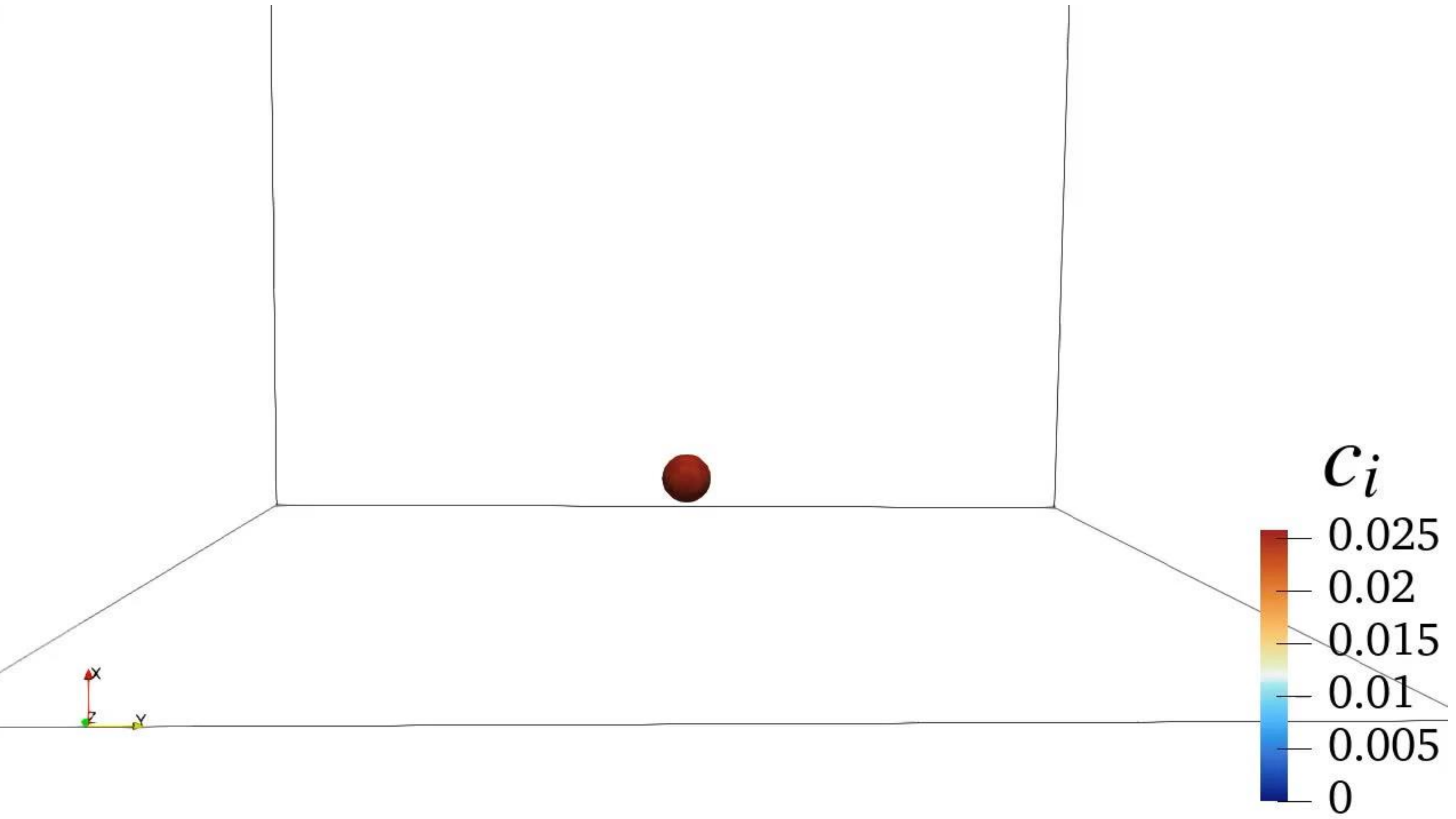
Rising bubble 3D

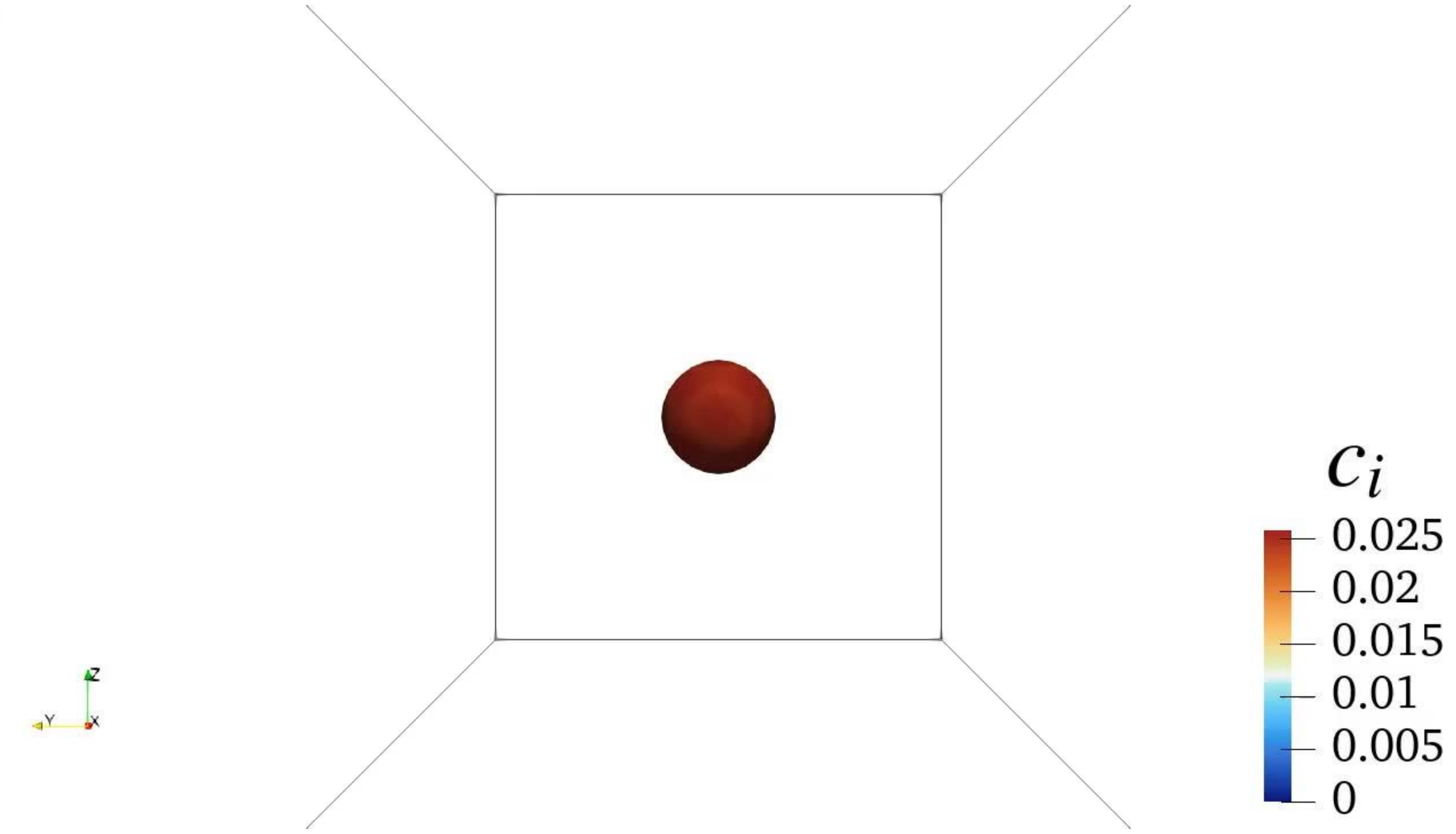
$\frac{\rho_l}{\rho_b} = 1000, \frac{\mu_l}{\mu_b} = 100, Bo = \frac{\rho_l g d_b^2}{\gamma_0} = 10, Ga = \frac{\rho_l d_b \sqrt{g d_b}}{\mu_l} = 100, Pe = \frac{d_b \sqrt{g d_b}}{D_i} = 100$ and $Ma = \frac{\beta \gamma_0}{\sqrt{g d_b} \mu_l}$

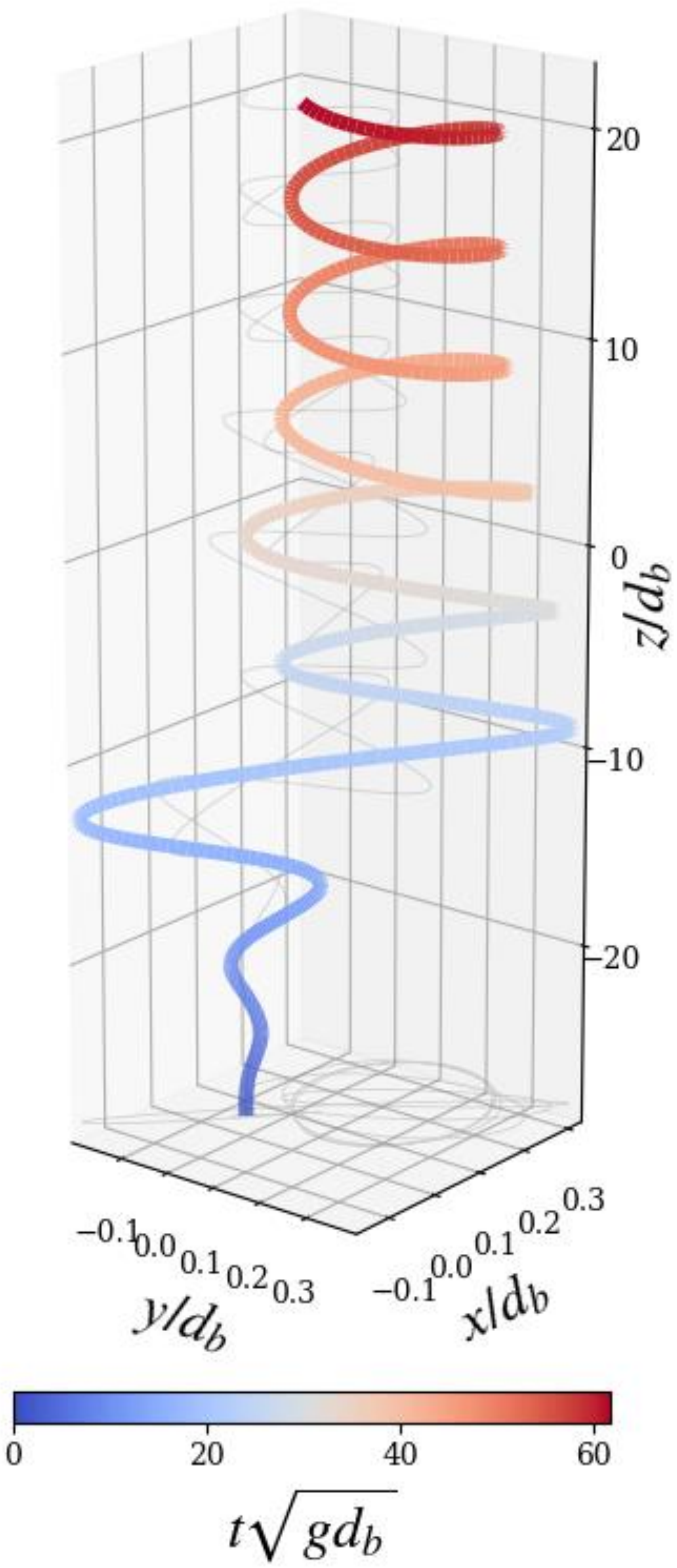


Rising bubble 3D

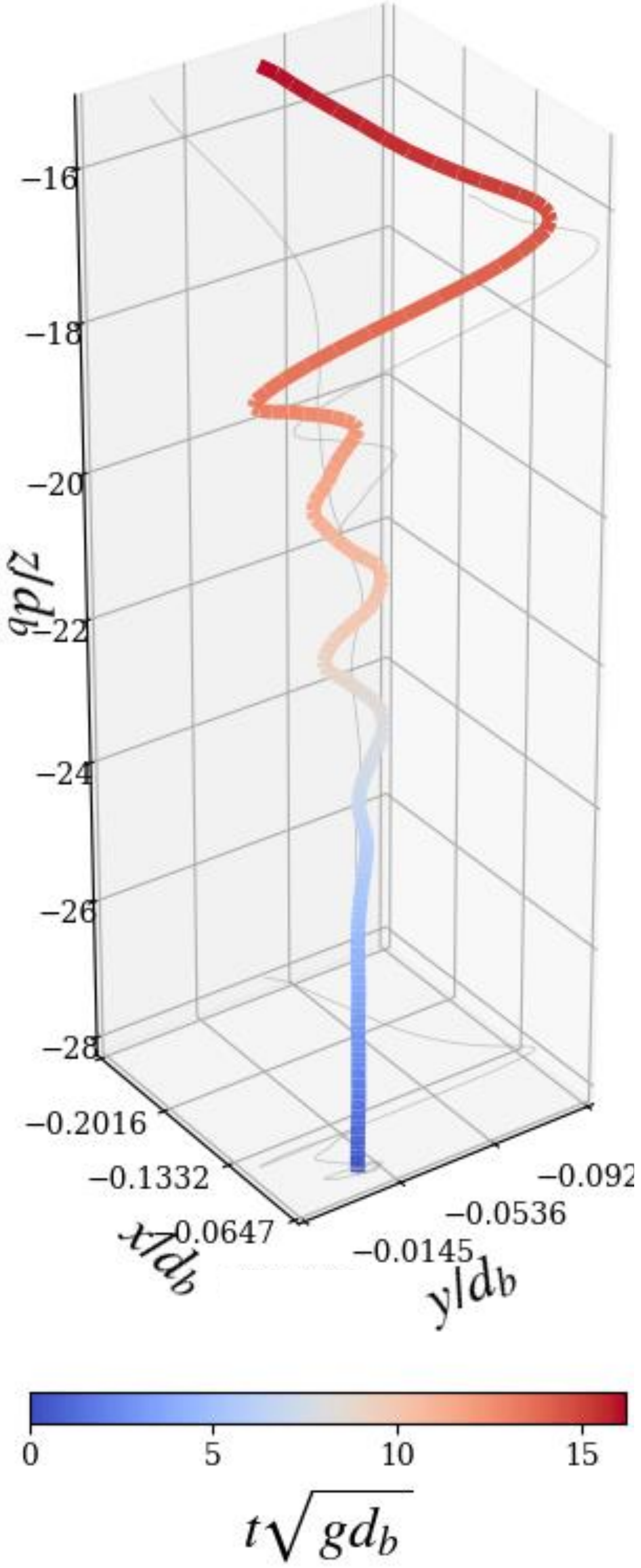
Trajectory instability



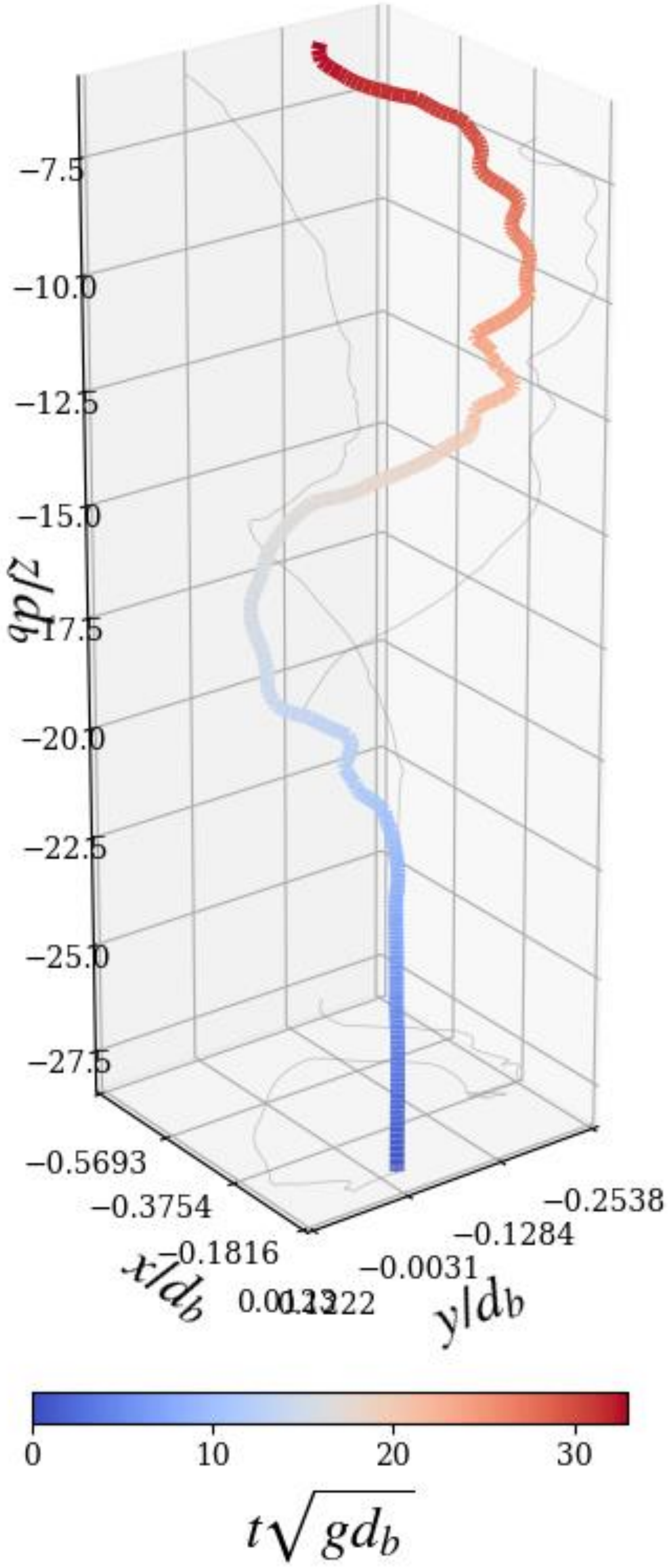




Without surfactant



Insoluble surfactant $Ma = 1$



Soluble surfactants Ma = 1, $r_d = 1, r_a = 0.01$

Fernández-Martínez et al. « *Transient bubble rising in the presence of a surfactant at very low concentrations* » International Journal of Multiphase Flow, (2025)

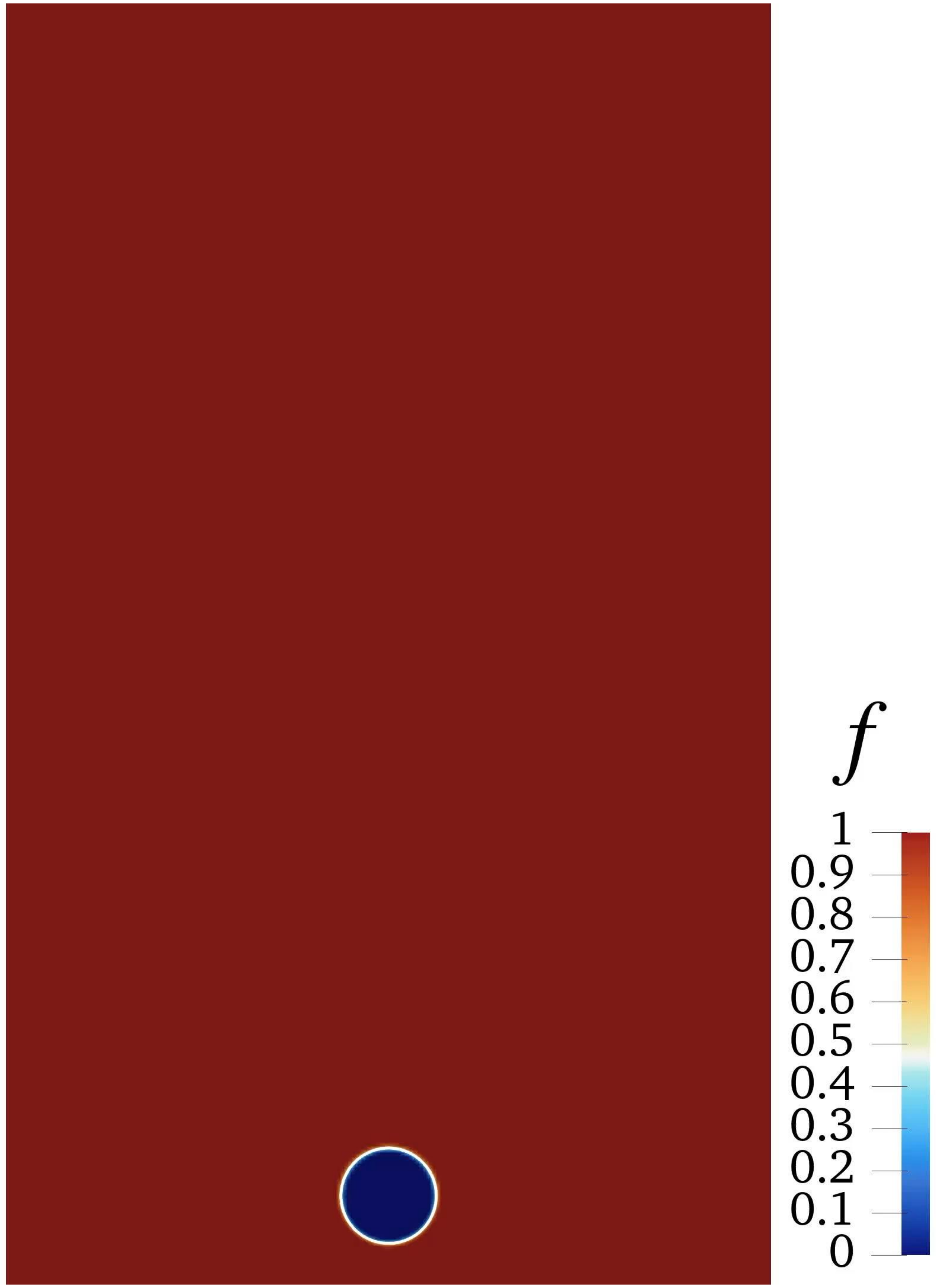
Rising bubble 2D Axi-symmetric

$$\mathrm{Bo} = \frac{\textit{gravitational effect}}{\textit{capillary effect}}$$

$$\mathrm{Ga} = \frac{\textit{gravitational effect}}{\textit{viscous effect}}$$

$$\mathrm{Pe} = \frac{\textit{convective effect}}{\textit{diffusive effect}}$$

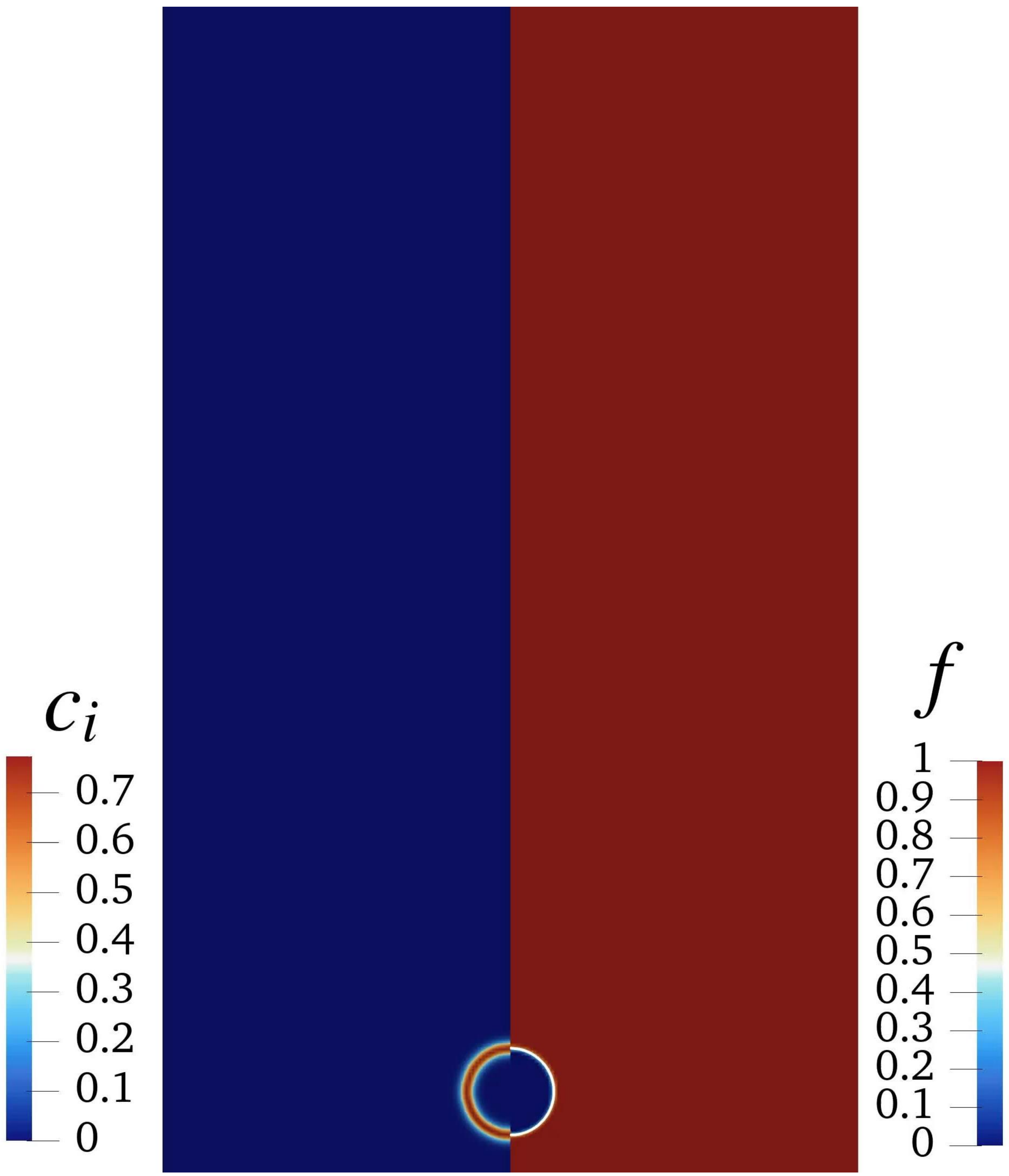
$$\mathrm{Ma} = \frac{\textit{shear force due to}\nabla\gamma}{\textit{diffusive effect}}$$



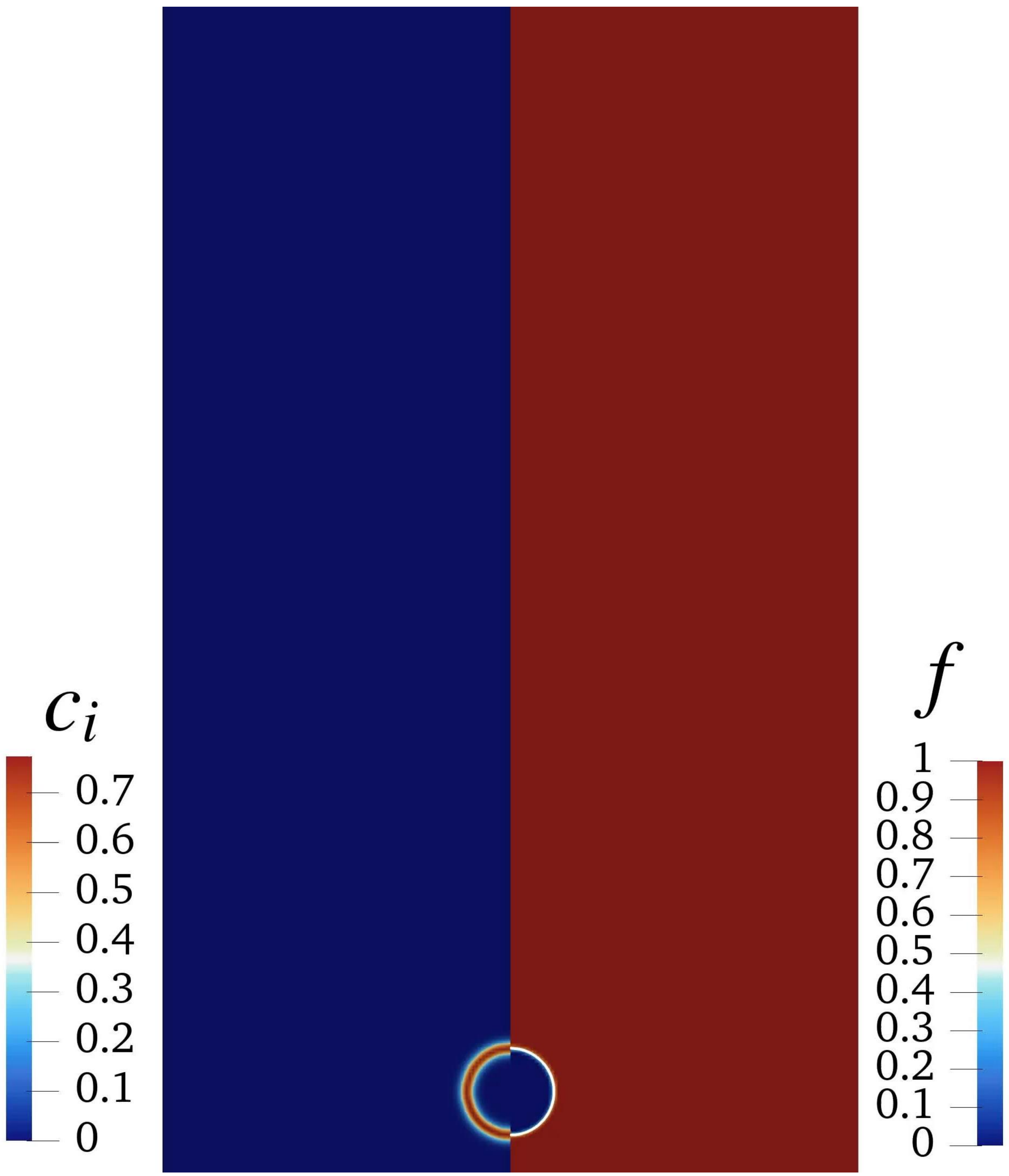
Without surfactants

Rising bubble 2D Axi-symmetric

It is insoluble surfactants in those simulations



With insoluble surfactants $Ma = 1$



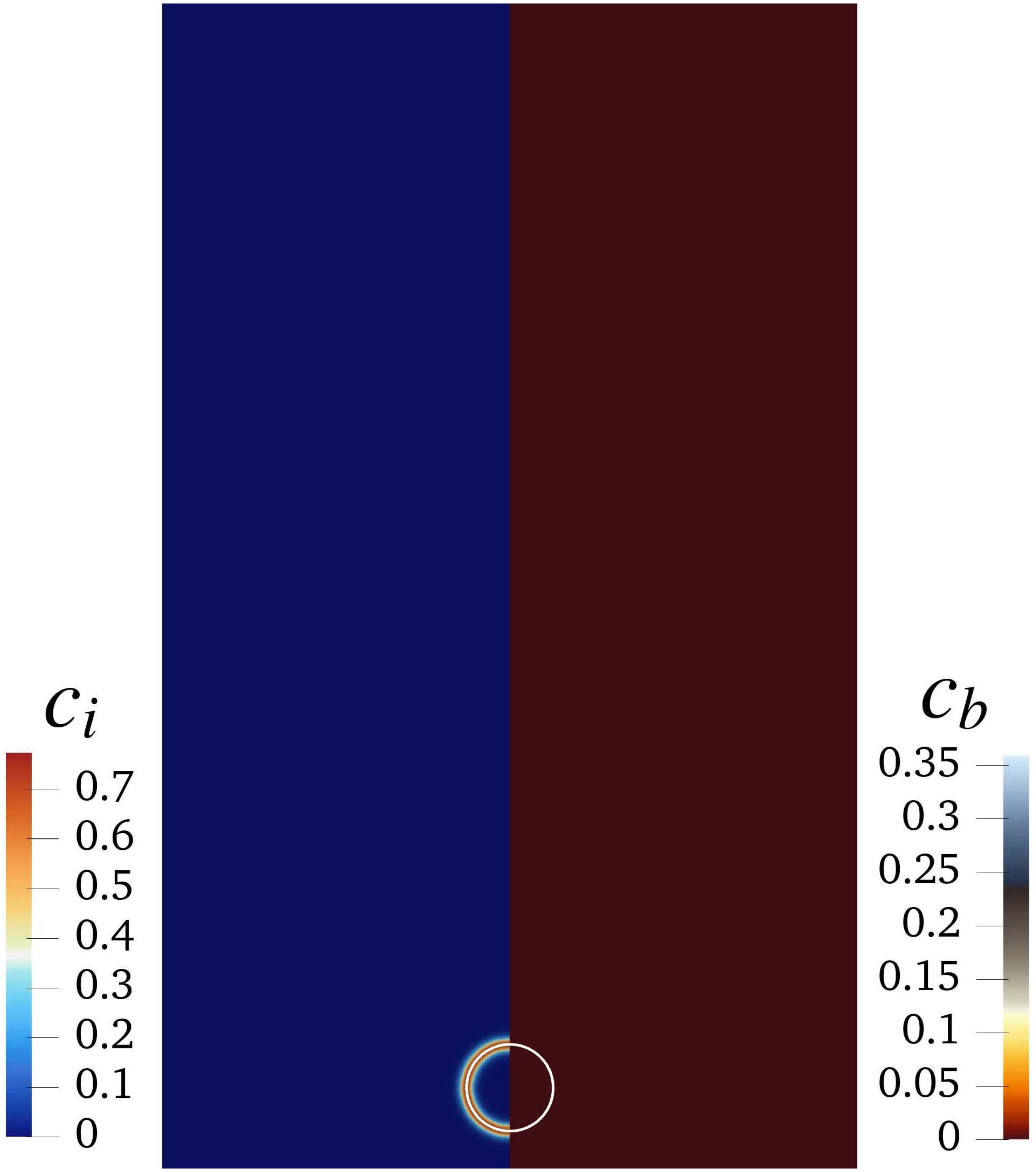
With insoluble surfactants $Ma = 20$

Rising bubble 2D Axi-symmetric

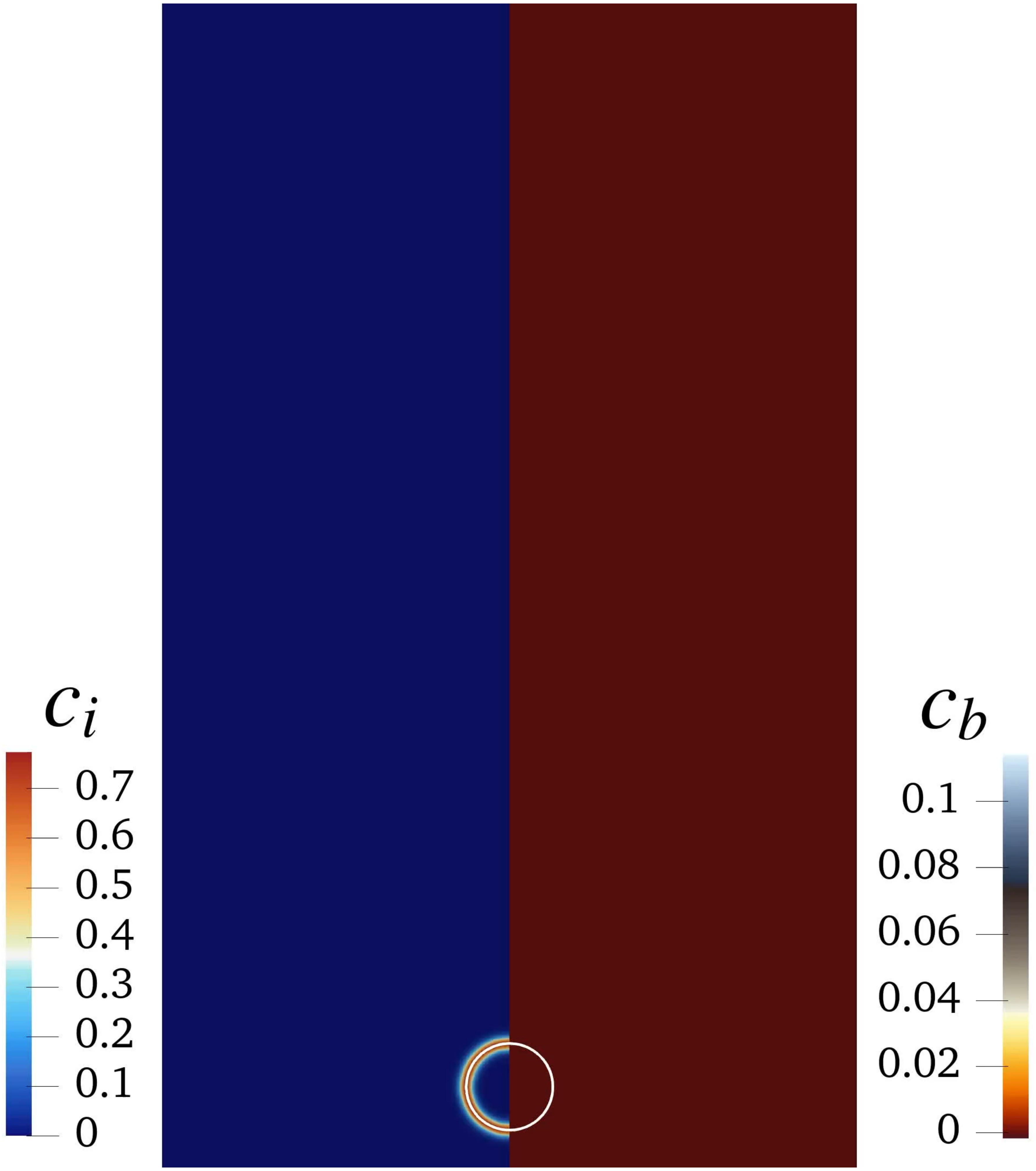
Influence of the Marangoni number on the deformation of the interface

Rising bubble 2D Axi-symmetric

Only the desorption r_d is considered in those simulations



With soluble surfactants $Ma = 1, r_d = 0.1$



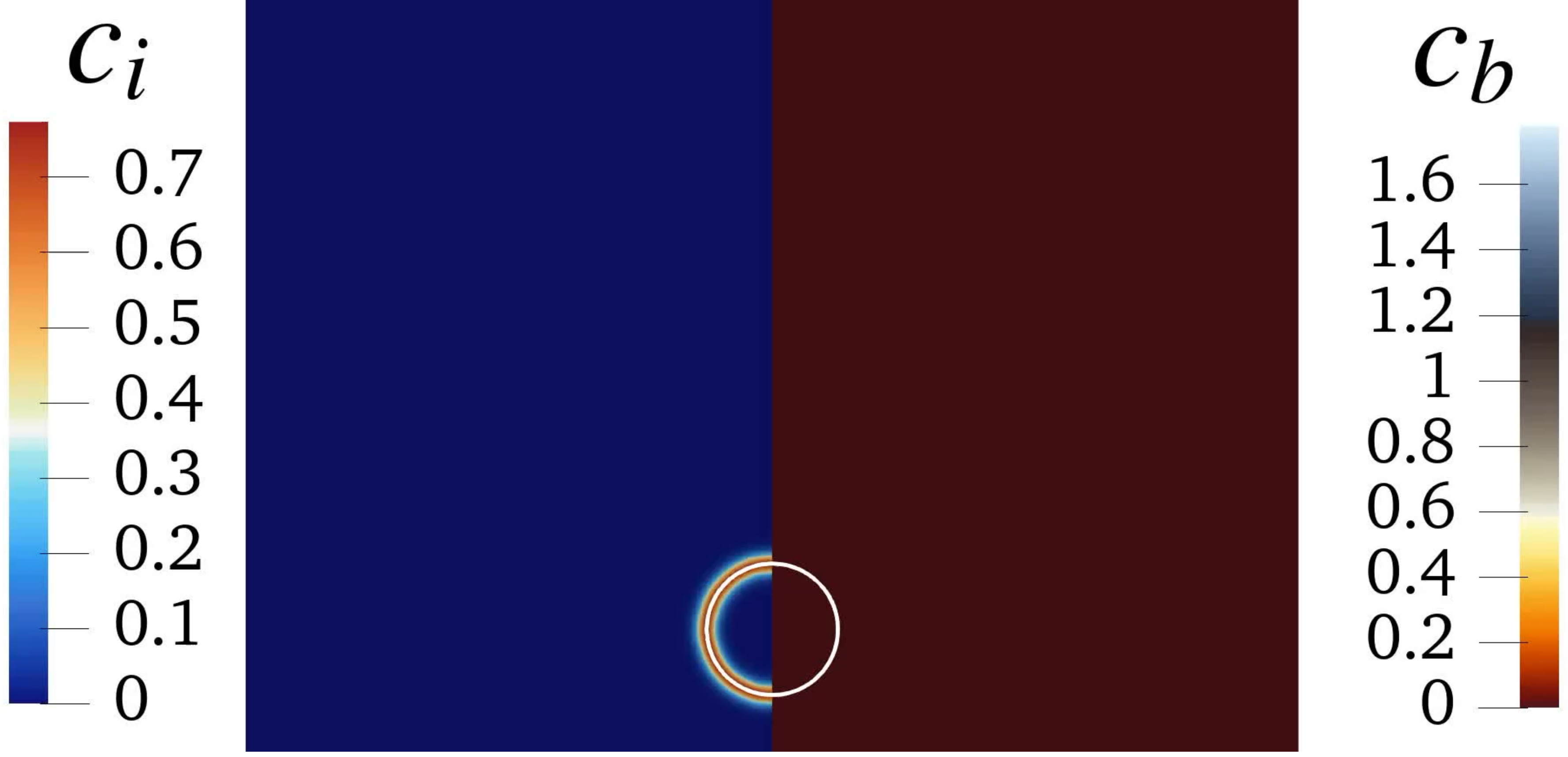
With soluble surfactant $Ma = 20, r_d = 0.1$

Rising bubble 2D Axi-symmetric

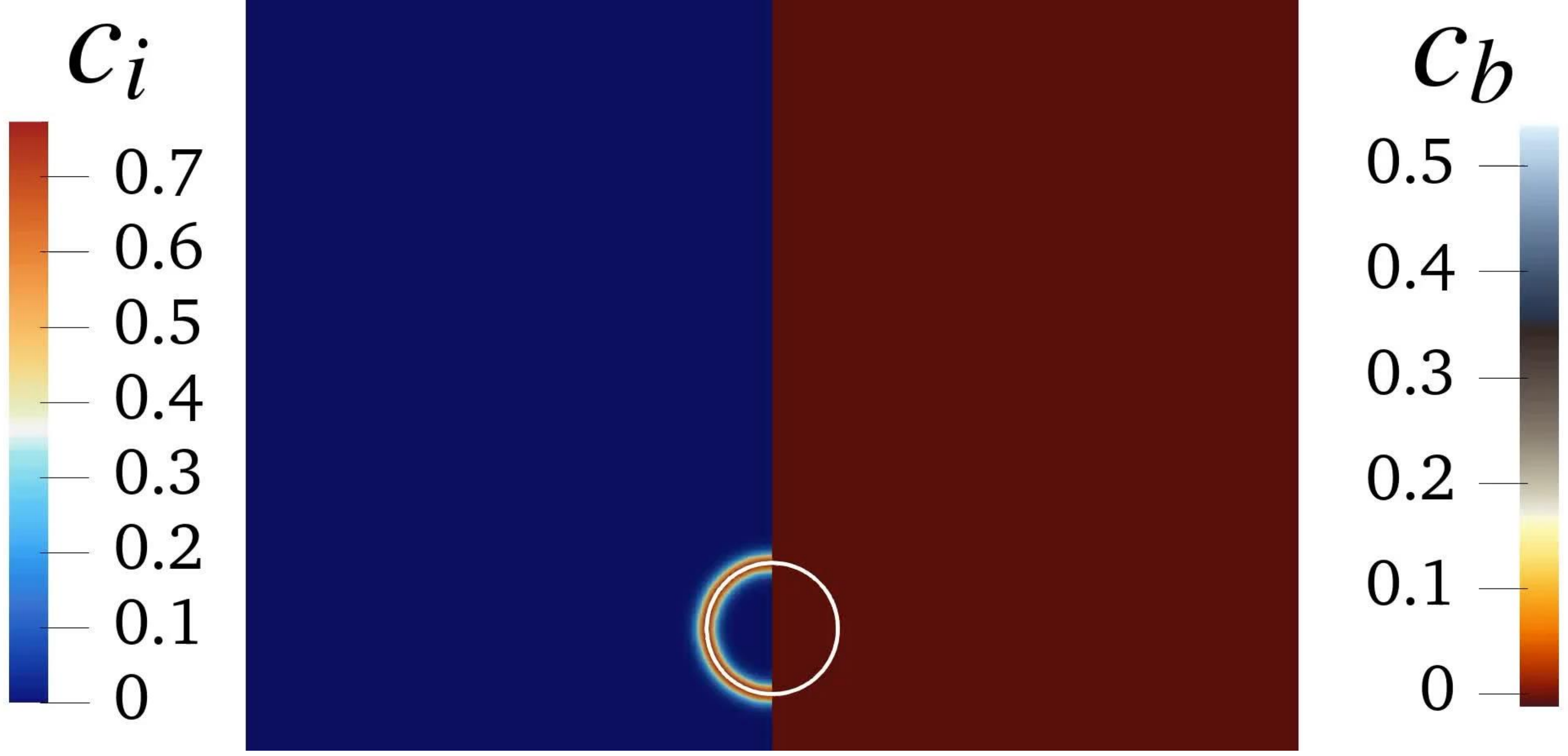
Influence of the desorption on the deformation of the interface

Rising bubble 2D Axi-symmetric

Only the desorption r_d is considered in those simulations



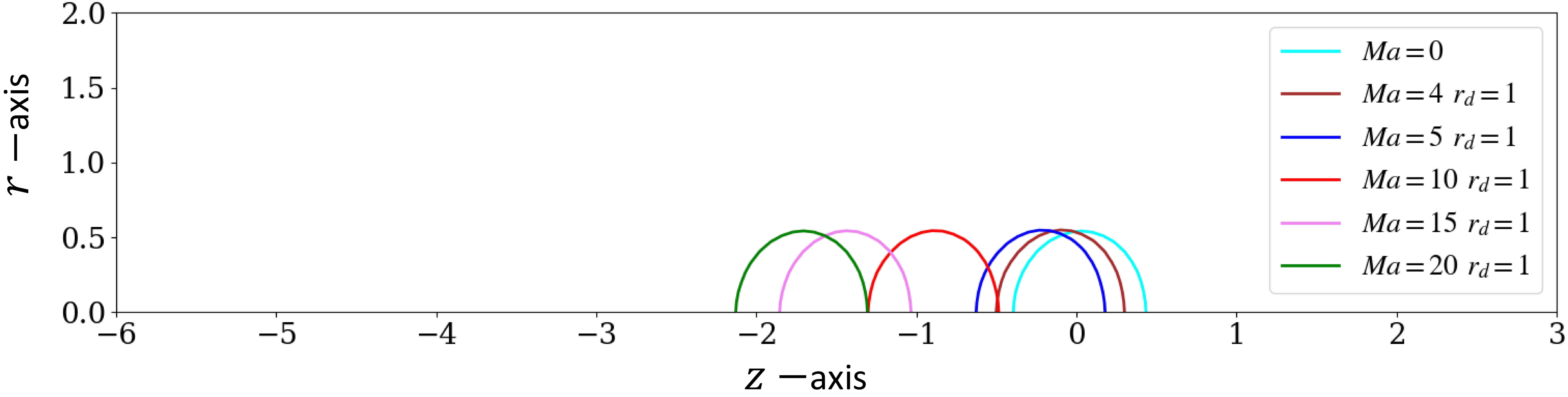
With soluble surfactants $Ma = 1, r_d = 1$



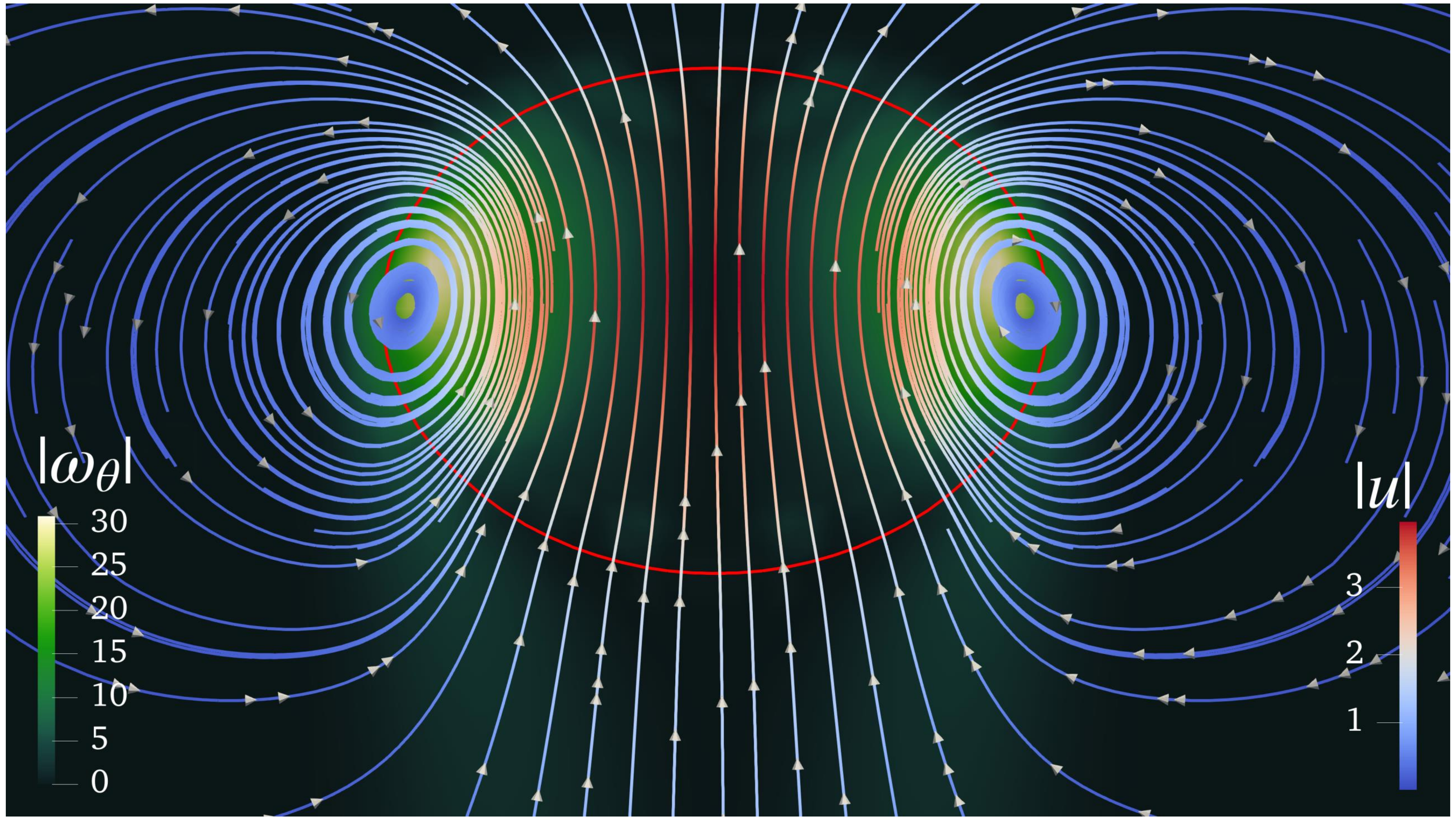
With soluble surfactants $Ma = 20, r_d = 1$

Rising bubble 2D Axi-symmetric

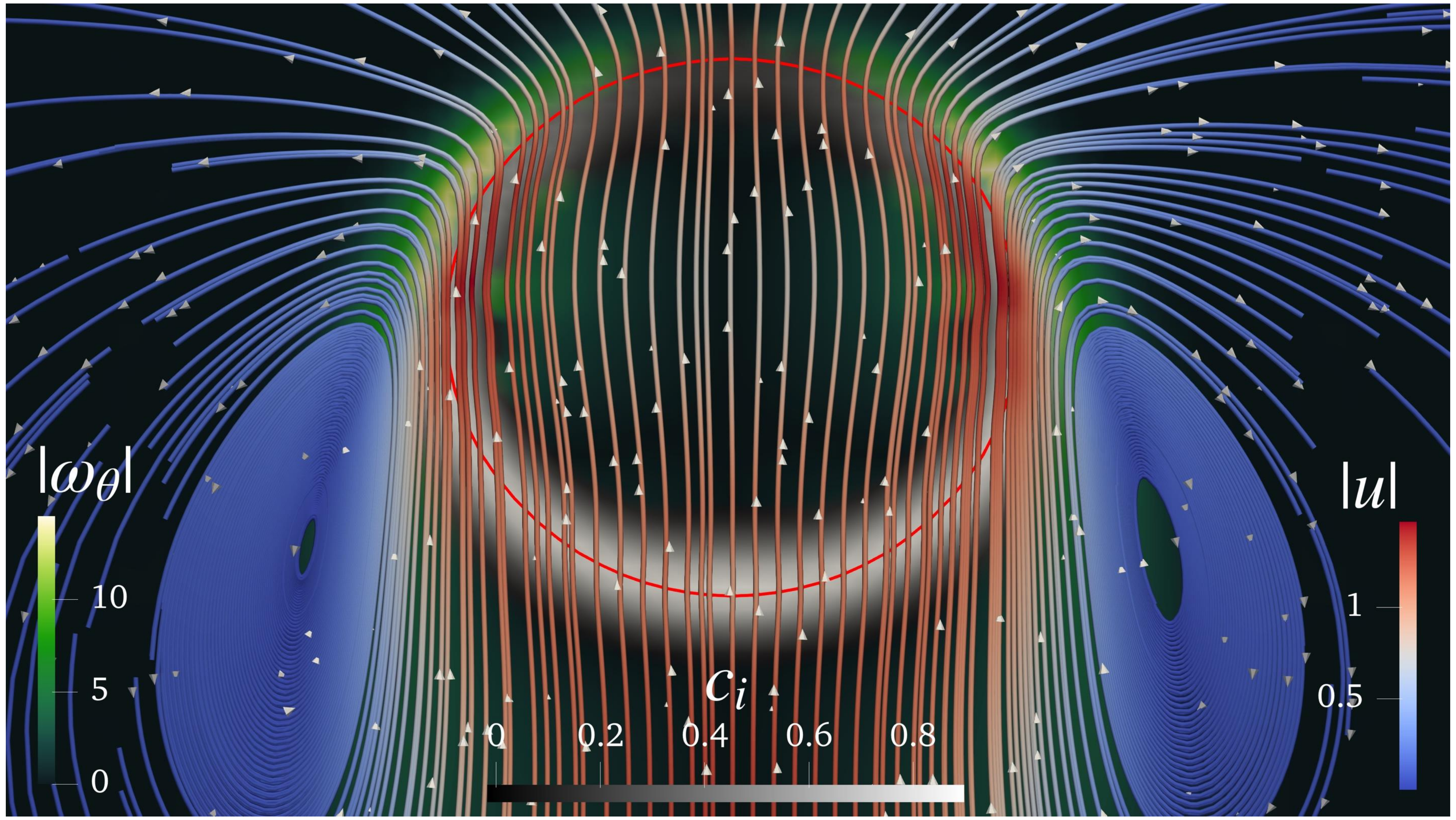
Influence of the desorption on the deformation of the interface



Rising bubble 2D Axi-symmetric



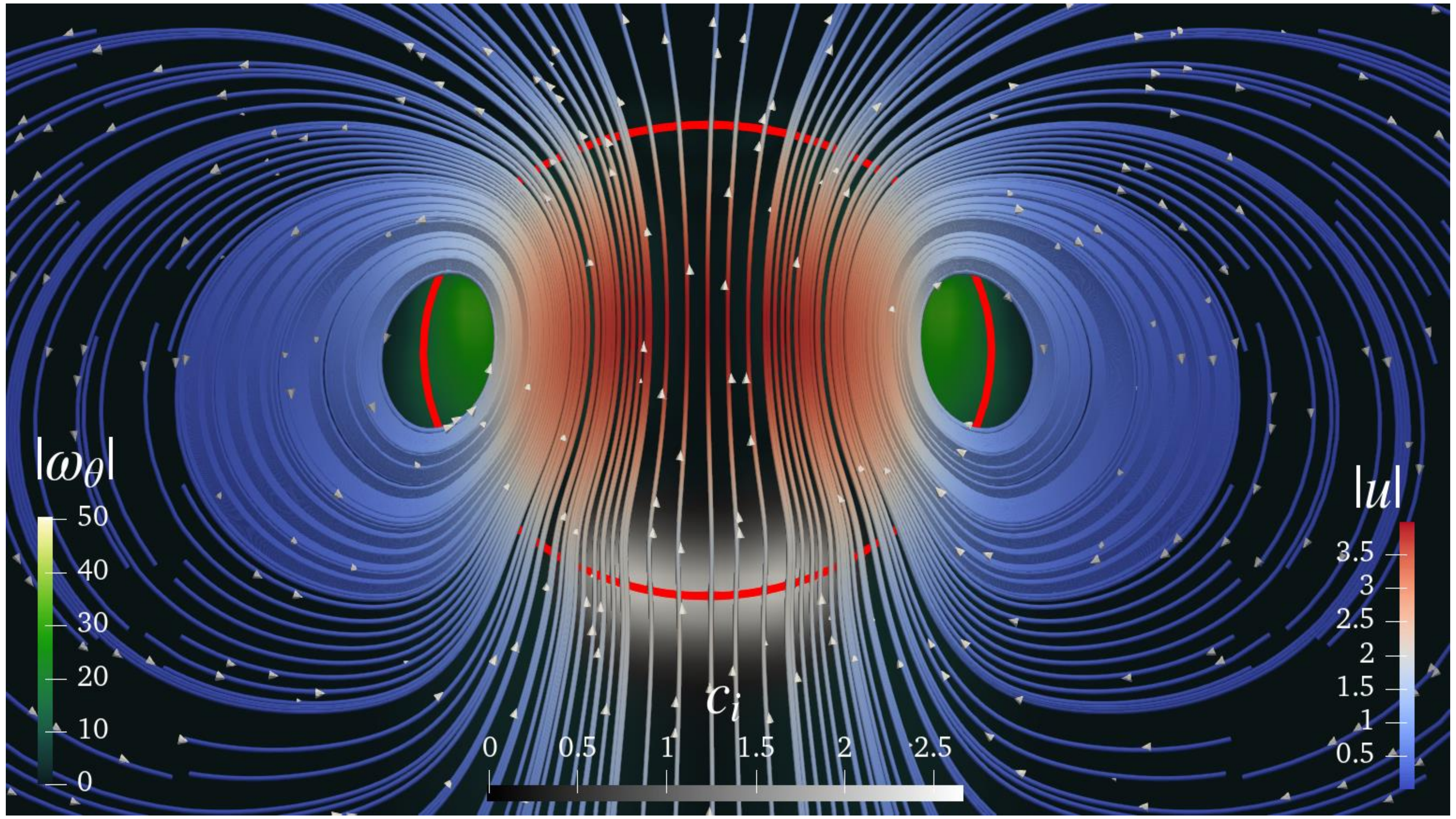
Without surfactants $Ma = 0$



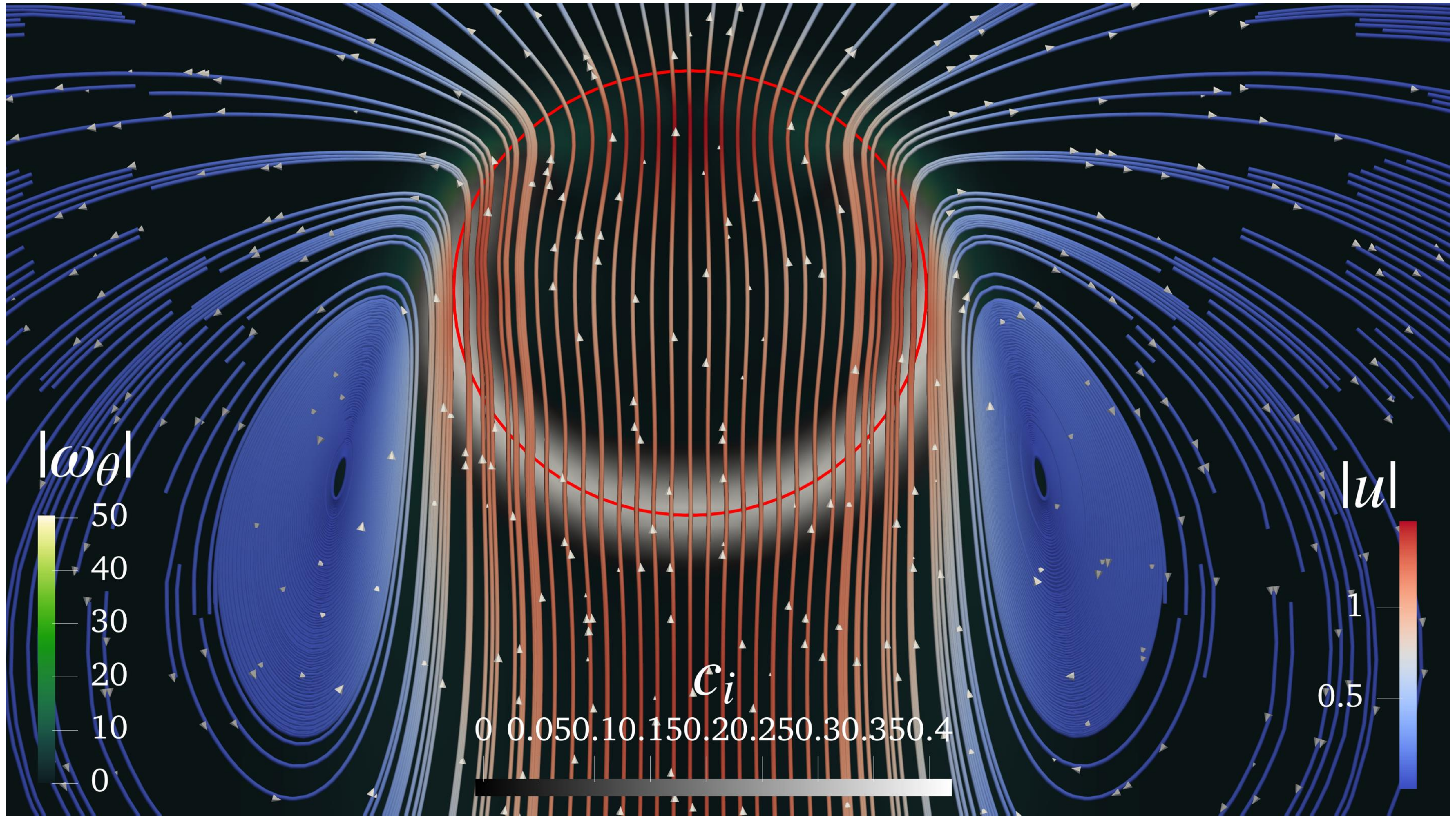
With insoluble surfactants $Ma = 20$

Rising bubble 2D Axi-symmetric

Only the desorption r_d is considered in those simulations



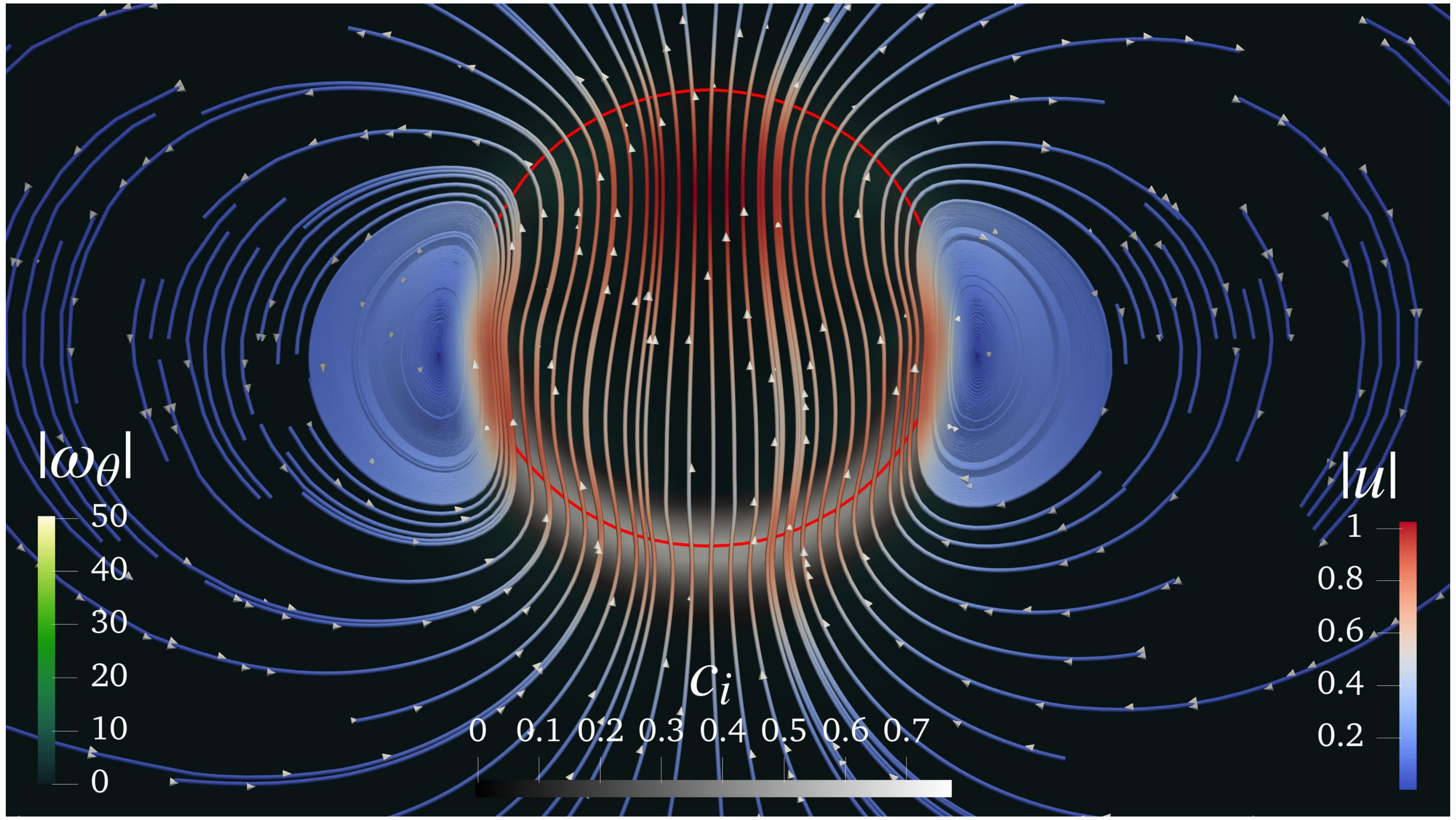
With soluble surfactants $Ma = 1, r_d = 0.1$



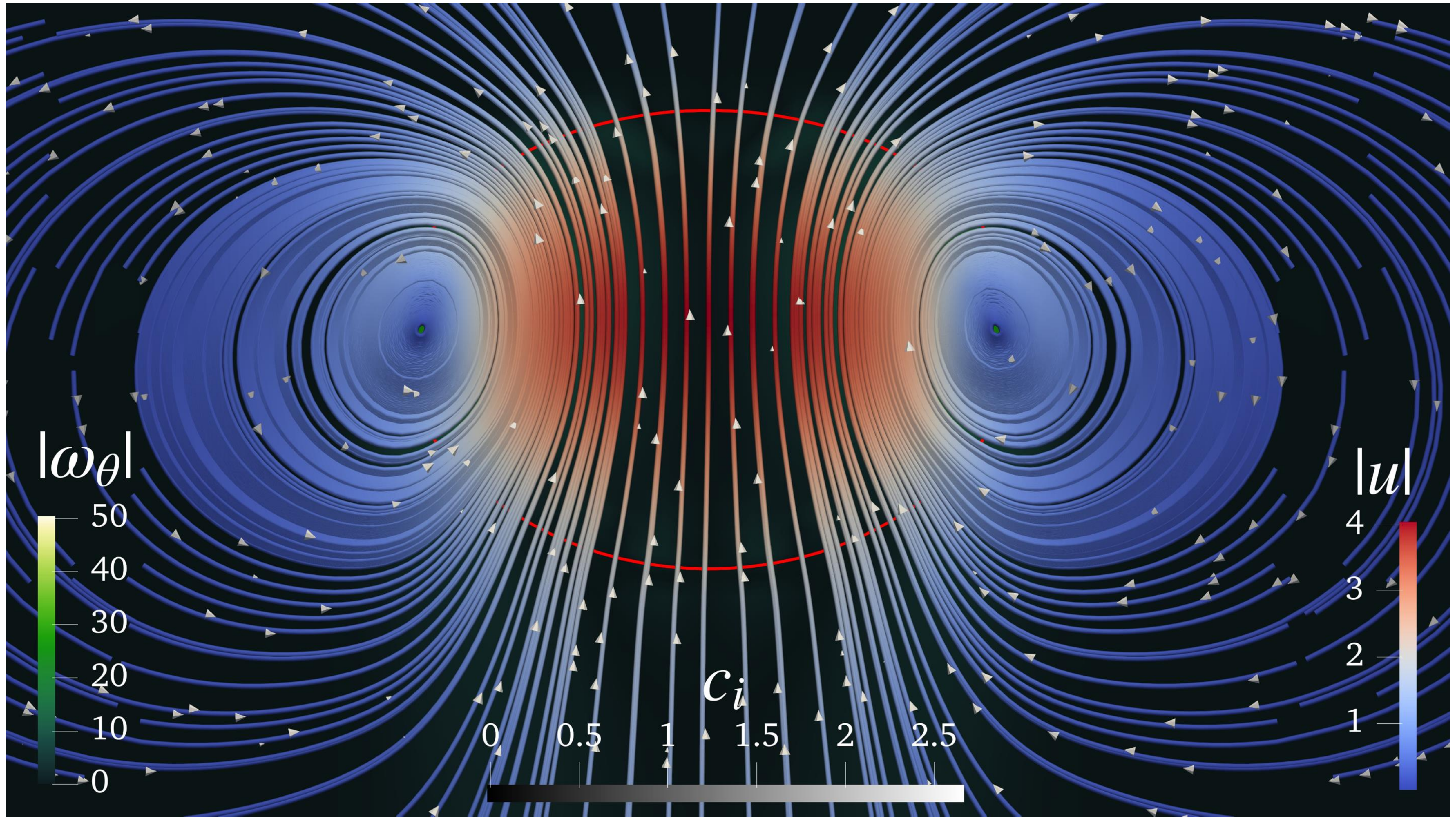
With soluble surfactants $Ma = 20, r_d = 0.1$

Rising bubble 2D Axi-symmetric

Only the desorption r_d is considered in those simulations



With soluble surfactant $Ma = 20, r_d = 1, \tilde{t} = 0.19$



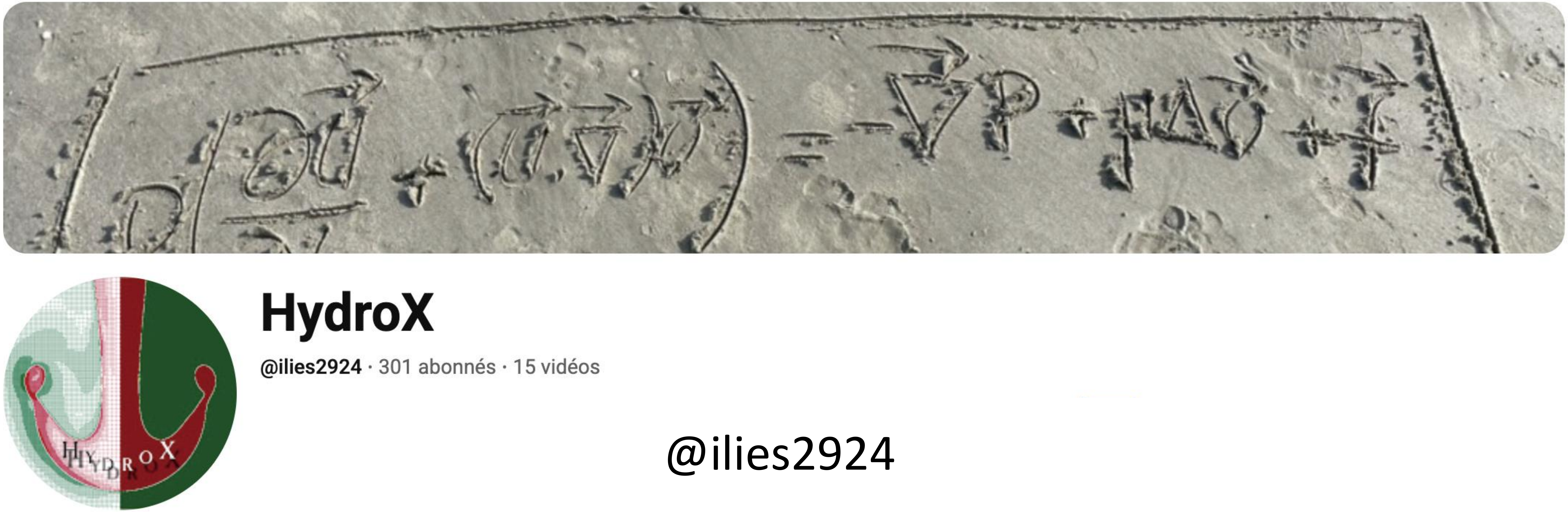
With soluble surfactant $Ma = 20, r_d = 1, \tilde{t} = 0.53$

Summarise/Next step

- Soluble surfactants for 2D/2D-Axis/3D configuration + AMR
- Open source sandbox/haouche - release soon

- Find some others test cases (with analytical solution)
- Use it for the soap film

Project: YouTube Channel



HydroX

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